TDDFT for Skyrme forces: role of current density in multipole giant resonances

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Abstract. Time-odd densities constitute an important part of the Skyrme functional as they restore its Galilean invariance violated by the effective-mass and spin-orbital terms. These densities do not contribute to ground state properties of even-even nuclei but may be important for the description of nuclear dynamics. As a particular case, we explore the influence of the time-odd current density $\vec{j}$ on E1, E2 and E3 giant resonances in ^{150}Nd. The analysis is done within the separable random-phase-approximation (SRPA) method with Skyrme forces SkT6, SkM*, SLy6, and SkI3. We examine relation of $\vec{j}$ to the effective masses and relevant parameters of the Skyrme functional and demonstrate strong influence of the current on the resonance properties for the forces with effective masses $m^*/m < 1$. The effect is fully determined by the force and essentially different for isoscalar (T=0) and isovector (T=1) cases. At the same time, it almost does not depend on the resonance multipolarity.

1 Introduction

Skyrme forces [1, 2] are widely used for description of diverse properties of atomic nuclei, in particular of nuclear dynamics (see, for recent reviews [3, 4]). However, even some principle features of these forces are not yet well clarified and need further analysis. In particular this concerns the role of the time-odd densities in the Skyrme functional. These densities are known to restore Galilean invariance of the functional, hence their fundamental role [5, 6]. Time-odd densities do not contribute to the static ground-state mean field of even-even nuclei but can affect the dynamics. The latter point is explored in the present paper.

We will outline time-odd densities in general and then concentrate on the role of the current density $\vec{j}$ in description of E1(T=1), E2(T=0,1) and E3(T=0,1) giant resonances (GR). The calculations are performed within the self-consistent separable RPA (SRPA) method [7–11] recently derived by our group. Due to factorization of the residual interaction, SRPA needs only a modest computational effort and so is quite effective for systematic exploration of complex nuclei. The method treats both spherical and deformed nuclei. It is self-consistent and does not need additional parameters. Due to the effective self-consistent procedure, SRPA demonstrate the accuracy of most involved methods. What is important for our aims, the method takes into account the contribution to the residual interaction of both time-even and time-odd densities. Coulomb contribution and pairing particle-particle channel are also included.

First systematic exploration of the impact of the current density to E1(T=1) and E2(T=0) GR was commenced in [10, 12]. Then the study was enlarged for a wider set of Skyrme forces and applied to a chain of Nd isotopes [13]. It was shown that $\vec{j}$-impact is generally strong and fully determined by the isoscalar and isovector parameters B_0 and B_1 of the Skyrme forces, responsible for the effective masses. The classification of the Skyrme forces into 3 groups, depending on the magnitude and sign of B_1, was proposed. It was demonstrated that the current impact does not depend on the shape and neutron number of the isotope, i.e. is the same for standard and exotic nuclei. This opens a possibility to explore the time-odd effects for standard nuclei and then transfer the results to exotic areas.

In the present paper we will demonstrate similarity of $\vec{j}$-impact for GR of *different* multipolarity λ. This finding is an additional important argument that contribution of the current density to $E\lambda$ GR is indeed mainly determined by the Skyrme force and insensitive to most of the nuclear and mode features.

2 Time-odd densities

2.1 General properties

The Skyrme functional [1] in the form [2, 5, 6, 14]

$$E = \int d\vec{r}(\mathcal{H}_{\rm kin} + \mathcal{H}_{\rm C}(\rho_p) + \mathcal{H}_{\rm pair}(\chi_q) + \mathcal{H}_{\rm Sk}(\rho_q, \tau_q, \vec{s}_q, \vec{j}_q, \vec{\Im}_q, \vec{T}_q) \; , \qquad (1)$$

includes kinetic, Coulomb, pairing and Skyrme terms respectively. Expressions for the first three terms are done elsewhere [8, 11, 12, 14]. The Skyrme part reads

$$\begin{aligned}
\mathcal{H}_{\rm Sk} = & \frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_q \rho_q^2 - \frac{b_2}{2}\rho(\Delta\rho) + \frac{b_2'}{2}\sum_q \rho_q(\Delta\rho_q) \qquad (2) \\
& + \frac{b_3}{3}\rho^{\alpha+2} - \frac{b_3'}{3}\rho^{\alpha}\sum_q \rho_q^2 + b_1(\rho\tau - \vec{j}^{\,2}) - b_1'\sum_q(\rho_q\tau_q - \vec{j}_q^{\,2}) \\
& - b_4\left(\rho(\vec{\nabla}\vec{\Im}) + \vec{s}\cdot(\vec{\nabla}\times\vec{j})\right) - b_4'\sum_q\left(\rho_q(\vec{\nabla}\vec{\Im}_q) + \vec{s}_q\cdot(\vec{\nabla}\times\vec{j}_q)\right) \\
& + \tilde{b}_4\left(\vec{s}\vec{T} - \vec{\Im}^2\right) + \tilde{b}_4'\sum_q\left(\vec{s}_q\vec{T}_q - \vec{\Im}_q^2\right) \; .
\end{aligned}$$

It involves time-even (nucleon ρ_q, kinetic-energy τ_q, and spin-orbital $\vec{\Im}_q$) and time-odd (current $\vec{j}_q$, spin $\vec{s}_q$, and vector kinetic-energy $\vec{T}_q$) densities, where q denotes protons and neutrons. The total densities (like $j = j_p + j_n$) are given in (2) without the index.

Both time-even and time-odd densities follow from the original Skyrme forces [1]. As was mentioned above, time-odd densities restore Galilean invariance of the functional, violated by velocity-dependent time-even densities τ_q and $\Im_q$ [5, 6]. So time-odd densities enter the functional only in the specific combinations with their time-even counterparts and do not lead to any new parameters. The latter is especially useful for even-even nuclei where Skyrme parameters can be fixed for the ground state by implementation of the time-even densities alone and then applied to nuclear dynamics involving time-odd densities as well.

The total set of six densities can be treated as the basic densities (ρ_q and $\vec{s}_q$), their momenta ($\vec{j}_q$ and $\vec{\Im}_q$) and kinetic energies (τ_q and $\vec{T}_q$) [5, 13]. Such presentation illustrates physical sense of the densities in terms of hydrodynamics. Besides it allows to interpret the Skyrme functional as some kind of the gradient expansion of the basic densities up to their second derivatives . Such expansion is reasonable for non-uniform densities, which is the case for $\vec{s}_q$ and ρ_q at the nuclear boundary [3].

2.2 Current density

Between time-odd densities, the current is most important for electric GR. Indeed, the spin density $\vec{s}_q$ is mainly relevant for magnetic modes and does not influence electric GR [10, 12]. The density $\vec{T}_q$ can also be neglected as its supplement $\Im_q^2$ is omitted in most of the Skyrme forces.

Contribution of $\vec{j}_q$ to the residual interaction is driven by the variation [8, 10]

$$\frac{\delta^2 E}{\delta \vec{j}_{q'}(\vec{r}')\delta \vec{j}_q(\vec{r})} = 2[-b_1 + b_1' \delta_{q,q'}]\delta(\vec{r}' - \vec{r}) \tag{3}$$

which is fully determined by the terms $\sim b_1, b_1'$ in the functional (2). In these terms, the current density adjoins the values $\rho\tau$ and $\rho_q\tau_q$ responsible for the effective masses. Hence, one may expect the correlation between effective masses and $\vec{j}_q$ in the GR dynamics.

To analyze this correlation, it is convenient to express the terms $\sim b_1, b_1'$ through the isoscalar and isovector densities $\rho_0 = \rho_n + \rho_p$ and $\rho_1 = \rho_n - \rho_p$ (the same for τ and $\vec{j}$). Then the sum of the these terms is transformed to the form [4]

$$B_0(\rho_0\tau_0 - j_0^2) - B_1(\rho_1\tau_1 - j_1^2) \tag{4}$$

where isoscalar and isovector contributions are decoupled and

$$B_0 = b_1 - b_1'/2, \quad B_1 = b_1'/2 \ . \tag{5}$$

For the symmetric nuclear matter, the isoscalar effective mass m^*/m and their isovector counterpart, the sum-rule enhancement factor $\kappa = (m_1^*/m)^{-1} - 1$ (where m_1^*/m is the isovector effective mass) are expressed via the new parameters as

$$(\frac{m^*}{m})^{-1} = 1 + \frac{2m}{\hbar^2}\bar{\rho}B_0, \quad \kappa = \frac{2m}{\hbar^2}\bar{\rho}(B_0 + B_1) \tag{6}$$

Table 1. Nuclear matter and deformation values for the Skyrme forces under consideration. The table represents the isoscalar (parameter B_0 and effective mass m_0^*/m) and isovector (parameter B_1, sum rule enhancement factor κ, and effective mass $m_1^*/m = 1/(1+\kappa)$) values, as well as the cartesian quadrupole moment Q_2 in ^{150}Nd. The experimental value of Q_2 are taken from [15].

Forces	B_0 [MeV fm^5]	m_0^*/m	B_1 [MeV fm^5]	κ	m_1^*/m	Q_2 [b]
SkT6	0	1.00	0	0	1.00	6.0
SkM*	34.7	0.789	34.1	0.531	0.653	6.2
SLy6	58.6	0.690	-26.0	0.250	0.800	5.8
SkI3	96.3	0.577	-64.0	0.246	0.802	5.9
exp.						5.3

where m is the bare nucleon mass and $\bar{\rho}$ is the density of the symmetric nuclear matter. Table 1 lists values (5) and (6) for the Skyrme forces used at the paper.

The velocity- and spin-dependent densities in the Skyrme functional should influence energy-weighted sum rules (EWSR) for electric GR [16, 17]. The most essential contributions are provided by the densities τ and $\vec{j}$ [17]. The former results in the effective mass. However, for isoscalar modes the τ and $\vec{j}$ contributions to EWSR fully compensate each other [17]. So, if we take $\vec{j}$ into account, then EWSR(T=0) again acquires the bare mass m and becomes

$$\mathrm{EWSR(T=0,\lambda>1)} = \frac{(\hbar \mathrm{e})^2}{8\pi \mathrm{m}}\lambda(2\lambda+1)^2\mathrm{A} < \mathrm{r}^{2\lambda-2} >_\mathrm{A} \quad . \tag{7}$$

The compensation between τ and $\vec{j}$ contributions is not complete for isovector modes [17] and so EWSR(T=1, $\lambda \geq 1$) retains the effective mass:

$$\mathrm{EWSR(T=1,\lambda=1)} = \frac{(\hbar e)^2}{8\pi m_1^*}9\frac{NZ}{A} \ , \tag{8}$$

$$\mathrm{EWSR(T=1,\lambda>1)} = \frac{(\hbar e)^2}{8\pi m_1^*}\lambda(2\lambda+1)^2 Z < r^{2\lambda-2} >_Z \quad . \tag{9}$$

For electric modes, contributions of spin-dependent densities $\vec{\Im}$, $\vec{s}$ and $\vec{T}$ to EWSR are usually neglected. This seems to be reasonable for $\vec{s}$. However, one should be careful with $\vec{\Im}$ and $\vec{T}$. Our calculations show that contribution of $\vec{\Im}$ to EWSR can be noticeable for the forces with large Skyrme parameters in the terms involving $\vec{\Im}$. In our study this is SkI3. For this force, removal of $\vec{\Im}$ from both mean field and residual interaction leads to increasing EWSR for E1(T=1) by 7-8%. Hence the same change in exhausting the estimation (8). The similar effect takes place for EWSR of other GR. However, their estimations (7) and (9) include the factors $< r^{2\lambda-2} >_A$ and $< r^{2\lambda-2} >_Z$ which are also affected by the removal of $\vec{\Im}$. As a result, $\vec{\Im}$ does not nearly influence exhausting (7) and (9). In general, $\vec{T}$-contribution can be significant for the forces with $\Im_q^2$ term in the Skyrme functional (the case of SkT6). In the present study we omit the term $\Im_q^2$ in SkT6 and so $\vec{T}$ as well.

3 Calculation Scheme

The study was performed with the representative set of four Skyrme forces (SkT6 [18], SkM* [19], SLy6 [20], and SkI3 [21]) for the deformed nucleus ^{150}Nd. Isovector and isoscalar characteristics of these forces are exhibited in Table 1. The forces somewhat overestimate the calculated moment of ^{150}Nd. However, this nucleus is rather soft and one hardly may expect here precise agreement with the experiment. In any case, this modest overestimation is irrelevant for our study.

The calculations were done within the SRPA approach [7–11] in the approximation of 5 input operators of a different radial dependence. Four operators were chosen following the prescription [8] and the fifth operator $r^{\lambda+2}Y_{\lambda+2,\mu}$ was added to take into account the multipole mixing of excitations with the same projection μ and space parity π. As was shown in our previous studies [8, 10, 12], such choice of the input operators makes the separable residual interaction sensitive to both surface and interior dynamics. Hence high accuracy of the calculations. In this paper, $4N_{op} = 20$ separable terms were used, where $N_{op} = 5$ is number of the input operators and factor 4 takes into account two options in isospin and time-parity. It worth noting that already two input operators are usually enough for the robust description of electric GR, even in deformed nuclei [10, 12]. The present set of input operators is even more safe.

GR were computed as the energy-weighted strength functions

$$S(E\lambda\mu;\omega) = \sum_{\nu} \omega_\nu M^2_{\lambda\mu\nu}\zeta(\omega-\omega_\nu) \tag{10}$$

smoothed by the Lorentz function $\zeta(\omega-\omega_\nu) = \varDelta/[2\pi((\omega-\omega_\nu)^2 + (\varDelta/2)^2)]$ with the averaging parameter $\varDelta$=2 MeV (such averaging was found to be optimal for the comparison with experiment and simulation of various smoothing factors). Here $M_{\lambda\mu\nu}$ is the matrix element of $E\lambda\mu$ transition from the ground state to the RPA state $|\nu>$, ω_ν is the RPA eigen-energy. The transition operator is

$$\hat{M}(\lambda\mu) = e_n^{eff}\sum_{i=1}^{N}(r^\lambda Y_{\lambda\mu})_i + e_p^{eff}\sum_{i=1}^{Z}(r^\lambda Y_{\lambda\mu})_i \tag{11}$$

where e_n^{eff} and e_p^{eff} are effective charges. They are (-Z/A, N/A) for E1(T=1), (1,1) for E2,E3(T=0), (1,-1) for E2,E3(T=1), and (0,1) for the proton response. We directly compute the strength function (10) and hence fully avoid determination of the numerous RPA eigen-states. This additionally reduces the computation time. As a result, SRPA calculations of one GR at a familiar laptop take less than one hour, as compared to weeks in the case of full RPA methods [22].

A large configuration space is used. It involves 247 proton and 307 neutron single-particle levels ranging from the bottom of the potential well up to $\sim +20$ MeV. All two-quasiparticle configurations for E1, E2 and E3 excitations up to the energy ~ 65 MeV are taken into account. The EWSR (7), (8) and (9) are exhausted by more than 90% for E1 and E2 and 80% for E3.

4 Results and Discussion

Results of the SRPA calculations are presented in Figs. 1-3. In Fig. 1 the resonances E1(T=1) and E2(T=0,1) in ^{150}Nd are exhibited for the set of four Skyrme forces. The quadrupole resonance is computed for the proton transition operator ($e_n^{eff} = 0$, $e_p^{eff} = 1$) and so includes both T=0 and T=1 branches. Right panels of the figure show, that except of SkT6, all the forces overestimate the E2(T=0) energy and the resulting upshift grows from SkM* to SkI3, i.e. with decreasing the isoscalar effective mass m^*/m of the forces. This trend agrees with the well known result that E2(T=0) GR prefers large m^*/m and so, the bigger m^*/m, the better E2(T=0) description.

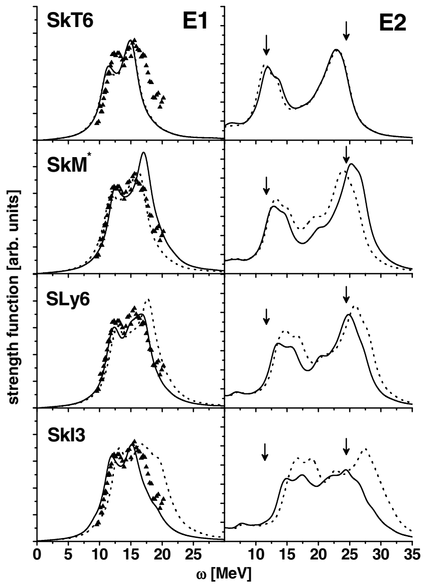

Figure 1. E1(T=1) and E2(T=0,1) giant resonances in ^{150}Nd, calculated with the Skyrme forces SkT6, SkM*, SLy6 and SkI3 for the cases with (solid curve) and without (dotted curve) contribution of the time-odd current. The strength is smoothed by the Lorentz weight with the averaging Δ=2 MeV. The experimental data for E1(T=1) [23–25] are depicted by triangles. The empirical estimations $\omega(E2, T=0) = 62A^{-1/3}$ MeV and $\omega(E2, T=1) = 130A^{-1/3}$ MeV for E2(T=0) and E2(T=1) resonance energies are marked the arrows.

As is seen from Fig. 1, the contribution of the current $\vec{j}$ downshifts the E2(T=0) energy for all the forces, except of SkT6, thus improving agreement with the estimation. The less m^*/m, the larger the current correction. For SkI3 this correction achieves an impressive value of $\sim$ 2 MeV. The correlation between the $\vec{j}$-contribution and m^*/m is explained by that both effects originate from the same isoscalar part $\sim B_0$ of the term (4) in the Skyrme functional. In fact both effects are determined by the isoscalar parameter B_0. This parameter systematically increases from SkT6 to SkI3, hence the trends. For SkT6 force, $B_0 = 0$ and so we have $m^* = m$ and vanishing the current contribution.

The situation with isovector E1 and E2 resonances is more complicated. It is seen from the left panels, that all the forces give in general acceptable agreement with the experiment for E1(T=1), though there are some visible deviations. The best agreement takes place for SLy6. This force has been fitted by the properties of asymmetric nuclear matter, hence good reproduction of isovector features. The other forces give noticeable disagreements: downshift and narrowing the resonance for SkT6 and SkI3 and an artificial right shoulder for SkM* (with $\vec{j}$-contribution).

What is remarkable, unlike the E2(T=0) case, the $\vec{j}$-impact for E1 has a different sign, depending on the force. Namely, the resonance energy is upshifted for SkM* and downshifted for SLy6 and SkI3. For SkT6 we again have a zero effect. Like for E2(T=0), these results are also driven by the term (4) but now by its isovector part $\sim B_1$. Indeed $\vec{j}$-impact is absent for SkT6 with $B_1 = 0$, gives upshift for SkM* with $B_1 > 0$ and leads to the downshift for SLy6 and SkI3 with $B_1 < 0$. Even magnitude of the shift correlates with the value of B_1 (see Table 1 for the comparison).

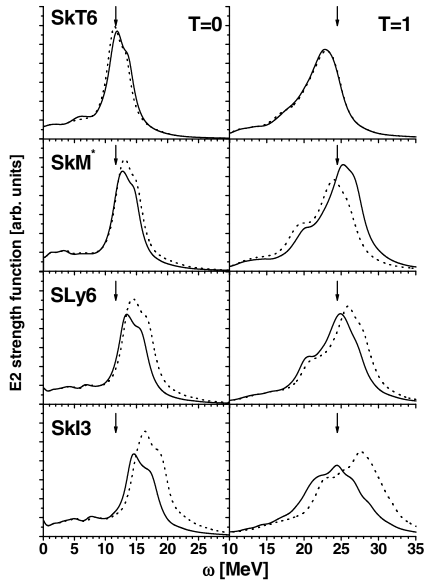

Figure 2. Isoscalar (left panels) and isovector (right panels) E2 giant resonances in ^{150}Nd, calculated with the Skyrme force SLy6 for the cases with (solid curve) and without (dotted curve) contribution of the time-odd current. The strength is smoothed by the Lorentz weight with the averaging Δ=2 MeV. The empirical estimations $\omega(E2, T = 0) = 62A^{-1/3}$ MeV and $\omega(E2, T = 1) = 130A^{-1/3}$ MeV for the resonance energies are marked the arrows.

Altogether this means that effective masses and $\vec{j}$-impact for E2(T=0) and E1(T=1) GR are related and determined by the force parameters B_0 and B_1. This conclusion agrees with the recent systematic exploration [13] involving 8 Skyrme forces and chain of 13 Nd isotopes. There the Skyrme forces were tentatively separated into 3 groups with $B_1 \sim 0$, $B_1 > 0$, and $B_1 < 0$. Following this classification, the forces SkT6, SkM* and SLy6,SkI3 should belong to the groups I, II and III, respectively. As is seen from Fig. 1, $\vec{j}$-impact in E1(T=1) can be negligible (I), harmful (II) and useful (III).

Right panels of Fig. 1 show that E2(T=1) resonance exhibits the same peculiarities as his dipole counterpart E1(T=1). In particular, its current impact is also determined by the isovector parameter B_1. So one may conclude that $\vec{j}$-impact does not depend on the GR multipolarity. Instead, it is mainly driven by the Skyrme force. This analysis remains to be valid for Fig. 2 where E2(T=0) and E2(T=1) GR are depicted separately. Moreover, we see the similar behavior for E3(T=0) and E3(T=1) resonances exhibited in Fig. 3.

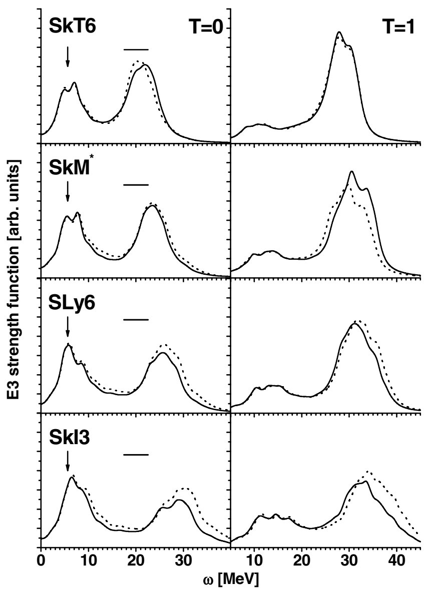

Figure 3. The same as in Fig. 2 for E3 giant resonances. The empirical estimations for the energies of isoscalar LEOR, $\omega(E3, T = 0) = 30A^{-1/3}$ MeV, and HEOR, $\omega(E3, T = 1) = (90 \div 120)A^{-1/3}$ MeV, are marked by the arrow and horizontal line, respectively.

The latter figure devotes a bit closer inspection. It is seen that both E3(T=0) and E3(T=1) are split into two branches, low-energy octupole resonance (LEOR) and high-energy octupole resonance (HEOR). These branches are determined by $\varDelta N = 1$ and $\varDelta N = 3$ particle-hole transitions, respectively, where N is the principle quantum shell number. Fig. 3 shows that we rather well describe the isoscalar LEOR. For the HEOR(T=0), the experimental data exhibit a wide dispersion, depending on the reaction and details of the experiment. For example, the resonance energy changes from $93A^{-1/3}$ MeV (recent (α, α') experiment [26]) to $110 \div 120A^{-1/3}$ MeV (systematic analysis of experimental data [27]). The corresponding uncertainty interval is marked in Fig. 3. It is seen that quality of HEOR(T=0) description is more or less the same as for E2(T=0). Namely, the HEOR(T=0) energy is somewhat overestimated and the deviation grows from SkT6 to SkI3. The right plots of Fig. 3 show that isovector LEOR and HEOR lie higher than their isoscalar counterparts. The experimental data for these GR are even more uncertain and so are skipped.

5 Conclusions

The influence of time-odd densities on multipole electric giant resonances is discussed and examined for the particular case of the current density $\vec{j}$. The calculations were done for E1(T=1), E2(T=0,1) and E3(T=0,1) resonances in the deformed nucleus ^{150}Nd for the Skyrme forces SkT6, SkM*, SLy6 and SkI3. The current contribution was found to be generally strong and fully determined by the isoscalar and isovector parameters B_0 and B_1 of the Skyrme forces, responsible for the effective masses. The contribution demonstrates essentially different behaviour for isoscalar and isovector GR but is insensitive to GR multipolarity.

Acknowledgments

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