Particle-vibration coupling versus tensor interaction in density functional theory

A. V. Afanasjev$^1$ and E. Litvinova$^{2,3}$

$^1$Department of Physics and Astronomy, Mississippi State University, MS 39762
$^2$Department of Physics, Western Michigan University, Kalamazoo, MI 49008-5252, USA
$^3$National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824-1321, USA

(Dated: September 18, 2014)

The energy splittings between the proton $1h_{11/2}$ and $1g_{7/2}$ states in the Sb ($Z = 51$) isotopes and the neutron $1i_{13/2}$ and $1h_{9/2}$ states in the $N = 83$ isotopes are analyzed within relativistic quasiparticle-vibration coupling (QVC) model. Although a common viewpoint is that an effective tensor interaction is needed to reproduce these splittings, we show, for the first time, that quasiparticle-vibration coupling also improves their description considerably. The remaining differences between the experiment and the QVC calculations point to a complex scenario in which both tensor interaction and quasiparticle-vibration coupling are needed to reproduce accurately the observed energy splittings. This scenario, however, requires a considerably weaker tensor interaction as compared with the previous estimates.

PACS numbers: 21.10.Jx, 21.10.Pc, 21.60.Jz, 27.70.+j, 27.70.+q

Density functional theory (DFT) is a well established theoretical tool for the description of the nuclei across the nuclear chart. For the majority of medium and heavy mass nuclei this is the only framework which can provide a microscopic description. However, it is not without drawbacks and significant efforts were dedicated to a search of missing terms and missing physics in its framework during last decade. One of possible candidates for such terms is the tensor interaction. It is well known that the tensor force is one of the important components of the bare nucleon-nucleon interaction. However, it is still an open question on whether the effective tensor force used in the DFT framework keeps a close resemblance with the original bare tensor force or not [1]. Moreover, the question of unambiguous signatures of the tensor force remains open [1]. For example, the fits of energy density functionals (EDF’s) to bulk nuclear properties (masses, radii) usually disfavor effective tensor interaction [1]; note that such fits are standard in the DFT. On the other hand, some possible indications of the presence of effective tensor interaction come from the analysis of the spectra of predominantly single-particle states in odd-mass nuclei; they are discussed in detail below. Possible manifestations of effective tensor force in the DFT framework have been recently reviewed in Ref. [1]. Although there is a general consensus that the tensor component has to be added to the DFT [1-7], the question about its strength is still not fully resolved.

Following Ref. [3], there were attempts to find a signature of the effective tensor force in the evolution of the single-particle states along the isotopic or isotonic chains. For example, the energy differences between the proton $1g_{7/2}$ and $1h_{11/2}$ states in the Sb ($Z = 51$) isotopes and the neutron $1i_{13/2}$ and $1h_{9/2}$ states in the $N = 83$ isotones were considered in Skyrme DFT calculations with the SLy5 functional in Ref. [3]. It was concluded that these energy splittings can be reproduced only when the tensor component is added to the functional. A similar investigation has been performed with the Gogny functionals in Ref. [3]. Again, the energy differences between the $1g_{7/2}$ and $1h_{11/2}$ states in the Sb isotopes with $N \geq 64$ can be reproduced only when effective tensor force is included. The tensor force has also been studied in relativistic Hartree-Fock approach in Ref. [9]. On one hand, the energy differences between the proton $1g_{7/2}$ and $1h_{11/2}$ states in the Sb ($Z = 51$) isotopes with $N \geq 66$ are only reproduced when the pion tensor coupling is included (although its strengh has to be reduced by a factor of two). On the other hand, extensive multi-parameter minimizations led to the conclusion that the optimal fit to bulk properties of infinite nuclear matter and spherical finite nuclei is achieved for the vanishing pion field, and, thus, no tensor force.

These investigations have been performed at the mean field level, although it is well known that particle-vibration coupling (PVC) affects the structure and the energies of the states of odd spherical nuclei [10, 12]. For example, it was recently demonstrated in Ref. [12] that relativistic PVC improves the description of the energies and wave functions of predominantly single-particle levels. In addition, Ref. [12] showed for the first time that PVC has an appreciable impact on the energy splittings of the spin-orbit and pseudospin doublets. The particle-vibration coupling accounts for long-range correlations between nucleons due to their exchange by quanta of collective excitations (phonons). Such a coupling introduces a time dependence into the nucleonic self-energy, which, in contrast, is treated in the static approximation in the mean-field theories.

It has been revealed in the studies of Refs. [3, 4] that the experimental data on the single-particle properties and, in particular, on spin-orbit splittings can be reproduced better at the DFT level if the tensor interaction is included and adjusted to this data. Thus, a compe-
tition of the effects coming from the PVC and tensor interaction may exist. For example, PVC decreases the splitting of the \(1f_{7/2} - 1f_{5/2}\) spin-orbit doublet of \(^{56}\)Ni by approximately 1.5 MeV. This doublet has been used in the definition of the strength of the tensor interaction in Refs. \([13, 14]\) where the effects of the PVC on its magnitude were neglected.

The main goal of this paper is to understand to which degree beyond mean-field effect, such as the particle-vibration coupling, can modify the conclusions coming from the studies of the tensor interaction kept at the mean field level. In order to achieve that, the energy differences between the proton \(1g_{7/2}\) and \(1h_{11/2}\) states in the Sb \((Z = 51)\) isotopes and the neutron \(1i_{13/2}\) and \(1h_{9/2}\) states in the \(N = 83\) isotones are studied within the QVC model developed in Ref. \([13]\).

![Diagram](image.png)

**FIG. 1.** (Color online) Pairing gaps used in the calculations as a function of particle number. The \(\Delta^{(5)}\) pairing gaps are extracted using experimental binding energies from Ref. \([14]\).

This model is an extension of the PVC model of Ref. \([10]\) and takes into account pairing correlations of the superfluid type in the quasiparticle-phonon coupling self-energy. The latter allows a proper description of the open-shell nuclei of interest. The QVC model has been successfully tested on the single-particle spectra in proton and neutron subsystems of \(^{116,120}\)Sn and applied to the superheavy nuclei \([13]\).

Monopole pairing force is used in our calculations. In order to study the dependence of the results of the calculations on the strength of pairing, two types of the parametrizations for the pairing gaps are employed. First, the calculations are performed with empirical pairing gap \(\Delta_{\text{emp}} = 12/\sqrt{A}\) MeV \([13]\), where \(A\) stands for the mass number. Second, the pairing gaps equal to five-point indicators \(\Delta^{(5)}\) \([16]\)

\[
\Delta^{(5)}(X) = \frac{(-1)^X}{8} [E(X + 2) - 4E(X + 1) + 6E(X) - 4E(X - 1) + E(X - 2)]
\]

defined for each nucleus under study from experimental odd-even mass staggerings are also used. Here \(X\) stands either for proton \(Z\) or neutron \(N\) numbers and \(E(X)\) is the (negative) binding energy of a nucleus with \(X\) particles. As shown in Ref. \([16]\), this indicator provides the best decoupling from mean-field effects in model calculations. For simplicity, we will refer such calculations as the "\(\Delta_{\text{emp}}\)" and "\(\Delta^{(5)}\)" ones.

The calculations have been performed with the NL3* covariant energy density functional (CEDF) \([17]\). This functional represents one of very few relativistic functionals the performance of which has been tested globally with respect of the ground state observables \([18]\) and systematically in the local regions of nuclear chart with respect of other physical observables (see Ref. \([19]\) and references therein). In the context of this paper, it is important that NL3* has been successfully used in the relativistic PVC studies of the spectra of odd spherical nuclei adjacent to doubly magic nuclei (such as \(^{100,132}\)Sn) and the impact of PVC on physical observables \([12]\).

Before considering the energy splittings of specific pairs of the states in odd-mass nuclei, it is necessary to understand how well the excitations energies and the electric multipole decay rates of the lowest lying vibrational states in the Sn and \(N = 82\) even-even nuclei are reproduced in the Relativistic Quasiparticle Random Phase Approximation (RQRPA). These characteristics play a decisive role in the QVC model: the nucleonic self-energy is a function of the phonons’ frequencies and quasiparticle-phonon coupling vertices (see, for instance, Eq. (5) of Ref. \([13]\)) while the latter are directly related to the decay rates. Thus, the accuracy of their description defines the quality of the description of the states with significant single-particle content in odd-mass nuclei. The excitation energies of the lowest \(2^+\) and \(3^-\) states and the corresponding reduced transition probabilities are shown in Figs. \([2a, 3a]\) while comparable accuracies are obtained in the "\(\Delta^{(5)}\)" calculations \((\text{Fig. } 3c)\). The level of agreement with experiment obtained in the
current calculations is at least comparable with the one obtained in earlier relativistic \cite{20} and non-relativistic \cite{21} QRPA calculations for the Sn isotopes. For example, it is comparable with the results of the Skyrme QRPA calculations obtained with the SkX functional, and it is either better or comparable [dependent on physical observable (E(2+) , E(3−), B(E2) or B(E3))] with the results obtained with SkM* and SLy4 (compare Figs.2 and 3 in the present paper with Figs. 3 and 9 in Ref. [21]). Our results are also close to the ones obtained in the relativistic QRPA calculations of Ref. [20] with the NL3 CEDF (compare Figs. 2 and 3 in the present paper with Figs. 8, 9, 11, and 12 in Ref. [20]).

Apart of the Z = 58, 60 nuclei, the excitations energies of the 2+ states in the N = 82 isotones are reasonably well reproduced in the model calculations (Fig. 2b). The results for Z = 58, 60 are affected by too big shell gap at Z = 58, which appear in many CEDF’s. It was shown in Ref. [22] that ρ-meson tensor coupling can reduce the size of this gap. The results for the reduced B(E2) transition probabilities are, nevertheless, close to experiment (Fig. 3b). Experimental excitation energies of the 3− states are overestimated for N ≤ 58 (Fig. 2a) because of the same reason as the 2+ energies, and only above this neutron number the results of the calculations come close to experimental data. It turns out that for the case of “Δ_{emp}” pairing the QRPA calculations of the 3− excitations in the Z = 64, 66 and 68 N = 82 isotones lead to the appearance of the Goldstone modes. Only for the pairing strength larger than some critical value the energies and the B(E3) values of the lowest 3− states have physical magnitudes. The critical value for the pairing gap is larger than the “Δ_{emp}” for the nuclei with Z = 64 − 68. Therefore, no meaningful calculations can be done for them within the QVC model.

In experiment, the energy splitting \( \Delta_{\epsilon_{\sigma}} = \epsilon(\pi h_{11/2}) - \epsilon(\pi g_{7/2}) \) between the lowest states of the Sb isotopes corresponding to the two nodeless single-proton \( h_{11/2} \) and \( g_{7/2} \) orbitals outside the closed Z = 50 core gradually decreases in the N = 54 – 62 isotopes and then rapidly increases for N ≥ 62 (Fig. 4h). The change of the energy splitting \( \Delta_{\epsilon_{\sigma}} \) on going from N = 62 to N = 82 is substantial (around 2.5 MeV). The CDFT calculations (performed at the mean field level) give \( \Delta_{\epsilon_{\sigma}} \sim 4 \text{ MeV} \) which is smoothly increasing with neutron number. This is definitely in contradiction with experiment. It is interesting that Skyrme DFT calculations with the SLy5 functional also fail to reproduce experimental data; the energy splittings obtained at the mean field level are on average around 3.25 MeV (see Fig. 1 in Ref. [3]). To cure this problem, the tensor interaction is added to the Skyrme EDF in Ref. [3]. The pion tensor coupling introduced into the relativistic mean field in Ref. [3] also brings the energy splitting \( \Delta_{\epsilon_{\sigma}} = \epsilon(\pi h_{11/2}) - \epsilon(\pi g_{7/2}) \) in Sn isotopes with N ≥ 66 to a good agreement with data, when a factor 0.5 is introduced in the corresponding coupling strength.

Our results clearly show that a large part of the corrections to the energy splittings and, in some cases, the whole effect comes from the QVC. Indeed, the experimental \( \Delta_{\epsilon_{\sigma}} \) splitting and its trend with neutron number is reasonably well reproduced in the QVC calculations for the N ≥ 68 Sb nuclei. Even in lighter nuclei the QVC improves the agreement between theory and experiment as compared with the CDFT results. Note that the im-
pact of differences in the pairing gaps employed in the calculations on the $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ splittings is relatively small (Fig. 3). However, this improvement due to QVC is not sufficient to fully reproduce experimental trend. On going from $N = 66$ to $N = 50$ the energies of the lowest $3^-$ states calculated in RQRPA increase (Fig. 2) and the impact of QVC on the $\Delta\epsilon_\pi$ decreases (Fig. 4). The latter is a consequence of well-established fact that the QVC self-energy is very sensitive to the energies of the lowest $2^+$ and $3^-$ phonons. Experimental data on low-lying octupole states in the $N = 50 − 60$ tin nuclei do not exist 23. However, the increase of theoretical $3^-$ energies on approaching $N = 50$ (Fig. 2c) indicates that the contribution of the corresponding terms to the QVC self-energy weakens. However, for the isotopes with $N = 62, 64$, in which the experimental characteristics of the lowest quadrupole and octupole phonons are reproduced reasonably well in the RQRPA calculations, the reduction of the $\Delta\epsilon_\pi$ splitting in the QVC calculations is only a half of the magnitude which is necessary to reproduce the data. This points out to the increase of the importance of other than QVC mechanisms. Unfortunately, the studies of the pion tensor coupling in CDFT in Ref. [3] and tensor interaction in Gogny DFT in Ref. [3] do not cover the tin isotopes with $N = 50 − 64$. As a result, it is not clear whether the accounting of these tensor couplings will improve the description of the $\Delta\epsilon_\pi$ splittings for these nuclei. The inclusion of tensor interaction in the Skyrme SLy5 functional does not resolve completely the problems in the description of the $\Delta\epsilon_\pi$ splittings in these nuclei (see Fig. 1 in Ref. [3]).

A similar situation is seen in the energy splitting $\Delta\epsilon_\nu = \epsilon(\nu_{13/2}) − \epsilon(\nu_{9/2})$ of the single-neutron $i_{13/2}$ and $h_{9/2}$ states outside the $N = 82$ core (Fig. 4b). In the Skyrme DFT, this splitting is reasonably well reproduced by the inclusion of the tensor interaction [3]. The CDFT mean-field calculations do not reproduce the observed splittings, but the accounting of the QVC improves the description of the experimental $\Delta\epsilon_\nu$ values with the biggest improvement seen in the middle of the shell (Fig. 4b). Similarly to the case of the Sb isotopes, Figs. 2b, d and 4b show that the best agreement between experiment and theory for the $\Delta\epsilon_\nu$ is achieved for the nuclei in which the calculated excitation energies of the lowest $2^+$ and $3^-$ states are close to experimental ones. Thus, the improvement in the description of these physical observables should improve the description of the splittings.

The comparison of our QVC results with the DFT ones obtained with non-relativistic Skyrme [3] and Gogny [8] functionals as well as relativistic [3] functionals indicates that both QVC and tensor interaction act in the same direction and reduce the discrepancies between theory and experiment for the $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ splittings. If to consider both effects combined, the strong impact from QVC on the discussed splittings suggests that the effective tensor interaction has to be considerably weaker as compared with earlier estimates.

Fig. 5 shows the spectroscopic factors $S$ of the states under investigation calculated within the QVC model and their evolution with the particle number compared to available data. One can see that near magic shell gaps these states are of predominant single-particle nature ($S \sim 0.8$). However, the spectroscopic factors $S$ of these states decrease on going away from the magic gaps indicating the increased coupling of the single-particle motion with vibrations. These trends correlate with the trends of the excitation energies of the lowest $2^+$ and $3^-$ vibrational states. Indeed, the energies of these vibrational states are the highest for the doubly magic nuclei and they are by a factor 2-3 smaller in open shell nuclei (see Fig. 2). As a result, the coupling with vibrations is weaker in doubly magic nuclei and stronger in open shell nuclei, which results in the reduced spectroscopic factors $S$ of the considered states in the nuclei away from the magic ones. The calculated spectroscopic factors and the general trend of their evolution with particle number (Fig. 5) are not very sensitive to the differences of the pairing gaps $\Delta^{(5)}$ and $\Delta^{\text{emp}}$ (Fig. 1).

It was deduced in Ref. [25] that the states of interest are almost single-particle in nature. Based on these results it was concluded in the DFT framework that proper description of the $\Delta\epsilon_\pi$ and $\Delta\epsilon_\nu$ splittings requires tensor interaction [3, 6, 0]. Recently, an alternative analysis of Ref. [20] has shown that the fragmentation of the $\pi h_{11/2}$ and $\pi h_{11/2}$ states is greater than in the study of Ref. [25]. These results support the conclusions of earlier analysis of Refs. [27−29] which were in contradiction with Ref. [25]. As compared to the experimental data of Ref. [20], our QVC calculations reproduce well the experimental spectroscopic factors of the $\pi g_{7/2}$ state in all experimentally studied Sb nuclei and the ones of the $\pi h_{11/2}$ state in the $N = 62, 64$ Sb isotopes (Fig. 5b) and somewhat overestimate the fragmentation of the latter state in the

![Fig. 4](image-url) (Color online) The energy splittings between the indicated states obtained in experiment, covariant density functional theory (CDFT) and QVC calculations. The results of the calculations with two pairing schemes are shown. Experimental data are taken from Ref. 23.
\( N = 66 - 74 \) Sb isotopes. However, the \(^{117}\text{Sb}\) data on the spectroscopic factors of the \( \pi g_{7/2} \) and \( \pi h_{11/2} \) states \(^{27}\) are well reproduced in the QVC calculations (Fig. 5). In addition, in agreement with our QVC calculations the older experimental data of Ref. \(^{28}\) (see analysis in Ref. \(^{29}\)) provides low spectroscopic factor \( S \approx 0.5 \) of the \( \pi h_{11/2} \) state in the mid-shell Sb isotopes. Strong fragmentation of the single-particle strength cannot be accounted for at the DFT level. This again weakens the conclusions of Refs. \(^3, 5, 9\) on the need of strong tensor interaction.

In conclusion, the role of the quasiparticle-vibration coupling on the energy splitting of specific pairs of the states in odd-mass nuclei has been investigated in the relativistic framework. We focus on the energy splittings between the proton \( 1h_{11/2} \) and \( 1g_{7/2} \) states in the Sb (\( Z = 51 \)) isotopes and the neutron \( 1i_{13/2} \) and \( 1h_{9/2} \) states in the \( N = 83 \) isotones which, according to the earlier studies within the DFT framework, can be described only when effective tensor interaction is introduced. Our analysis clearly indicates that both QVC and tensor interaction act in the same direction and reduce the discrepancies between theory and experiment for the \( \Delta \epsilon_{\pi} \) and \( \Delta \epsilon_{\nu} \) splittings. As a consequence of this competition, the effective tensor force has to be considerably weaker as compared with earlier estimates. These results also show that the definition of the strength of the tensor interaction by means of the fitting to the energies of the dominant single-quasiparticle states in odd-mass nuclei is flawed without accounting for the effects of QVC.

This work has been supported by the U.S. Department of Energy under the grant DE-FG02-07ER41459, by the U.S. National Science Foundation under the grants PHY-120486 and PHY-1404343 and by the NSCL.

\[ \text{FIG. 5. (Color online) Spectroscopic factors } S \text{ of the states under study as a function of neutron and proton numbers. Experimental data are taken from Ref. \(^{28}\). No experimental data are available for the } N = 83 \text{ isotones.} \]

\[ \text{(a) } S_{5/2}^{\pi} - \Delta_{\text{emp}}, \quad S_{5/2}^{\pi} - \Delta_{\text{exp}}, \quad S_{11/2}^{\pi} - \Delta_{\text{emp}}, \quad S_{11/2}^{\pi} - \Delta_{\text{exp}}. \]

\[ \text{(b) } S_{5/2}^{\nu} - \Delta_{\text{emp}}, \quad S_{5/2}^{\nu} - \Delta_{\text{exp}}, \quad S_{11/2}^{\nu} - \Delta_{\text{emp}}, \quad S_{11/2}^{\nu} - \Delta_{\text{exp}}. \]