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Mean-field study of single-particle spectra evolution in $Z = 14$ and $N = 28$ chains

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We study the mechanisms that reduce the proton $1d_{3/2}$-$1d_{5/2}$ spin-orbit splitting and the neutron $1f_{7/2}$ subshell closure in ^{42}Si. We use various self-consistent mean-field models: nonrelativistic Skyrme-Hartree-Fock and relativistic density-dependent Hartree-Fock. Special attention is devoted to the influence of a tensor component in the effective interaction. It is found that the tensor force indeed governs the reduction of the $1d$ proton spin-orbit splitting. On the other hand, the reduction of the neutron $1f_{7/2}$ subshell closure is not clearly related to the tensor force.

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I. INTRODUCTION

With the progress that has been made in experimental studies of single-particle nuclear spectra, it has become clear that the single-particle levels undergo modifications when the neutron number N or proton number Z changes. From the experimental side, these studies are a difficult task, because the nuclei involved are generally short-lived and their production rate can be low. It is important to have in parallel theoretical models which may serve as guidelines for exploring the evolution of nuclear properties with N and Z numbers. A recent example is the work of Ref. [1], which has drawn attention to the possible effects of the neutron-proton tensor force on single-particle spectra along an isotopic or isotonic chain. This has triggered a number of experimental [2,3] and theoretical [4–7] works exploring this issue.

In the present work, we would like to use the self-consistent mean-field approach to analyze two findings based on experimental data complemented by a shell model analysis [2,3]: (1) the shrinkage of the proton spin-orbit splitting $1d_{3/2}$-$1d_{5/2}$ in the $Z = 14$ isotopes when going from $N = 20$ (^{34}Si) to $N = 28$ (^{42}Si); and (2) the quenching of the neutron shell closure gap $2p_{3/2}$-$1f_{7/2}$ when going along the isotonic chain $N = 28$ from $Z = 20$ (^{48}Ca) to $Z = 14$ (^{42}Si). Our analysis is based on both the nonrelativistic Hartree-Fock-BCS (HF-BCS) approach with Skyrme-type interactions [8] and the relativistic Hartree-Fock-BCS (RHF-BCS) approach [9]. Our aim is to discuss, among other things, the effects of the tensor component of the two-body effective interaction. The HF-BCS model is well suited for that purpose with the several Skyrme-type tensor forces proposed recently. On the relativistic side, the widely used relativistic mean-field (RMF) model cannot help, because it is just a Hartree approximation in which a tensor component in the interaction would have no effect. Therefore, we use in our analysis the RHF model where exchange (Fock) terms are kept and the pion-induced tensor interaction can play its role [10].

This paper is organized as follows. In Sec. II, we briefly give the main ingredients of the two models used in this analysis, namely, the nonrelativistic HF-BCS model with a Skyrme type interaction and the relativistic RHF-BCS model with density-dependent effective Lagrangians. In Sec. III, the results obtained for the $Z = 14$ isotopic chain and the $N = 28$ isotonic chain of nuclei are discussed. Conclusions are drawn in Sec. IV.

II. SELF-CONSISTENT MEAN-FIELD MODELS

We assume a spherical symmetry description of the nuclei studied here. Although this is a strong assumption for some nuclei of the isotopic and isotonic chains that we consider, it allows us to more easily gain insight into the role of separate parts of the mean field such as the central and spin-orbit potentials.

A. HF-BCS mean field with Skyrme interaction

The Skyrme-HF model is widely used, and we refer the reader to Ref. [8] for the notations of the present work as well as for the effective interaction SLy5 used here for generating the self-consistent mean field. In addition to the usual central and spin-orbit components of the Skyrme interactions (represented here by the SLy5 parametrization), we want to study the possible effects of a tensor component of the Skyrme force. This component was introduced in earlier versions of the Skyrme force [11–13], but it is only recently that attention has been focused on its effects on single-particle spectra in spin-unsaturated nuclei.

Along the chain of $N = 28$ isotones ($Z = 14$ isotopes), the proton-proton (neutron-neutron) pairing correlations will play a role, and they are treated in the BCS approximation [14] using a zero-range, density-dependent pairing interaction of the form

$$V^{(n\,\mathrm{or}\,p)} = V_0^{(n\,\mathrm{or}\,p)}\left(1 - \frac{\rho(\boldsymbol{R})}{\rho_0}\right)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2), \qquad (1)$$

where $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$, $\rho_0 = 0.16\ \mathrm{fm}^{-3}$ is the nuclear matter saturation density, and $V_0^{(n\,\mathrm{or}\,p)}$ is fitted for each chain to reproduce the empirical two-neutron (two-proton) separation energies. The pairing window contains the orbitals of the $1p$, $2s$-$1d$, and $2p$-$1f$ shells.

The effect of a tensor component in the Skyrme interaction is very simply described by a modification of the coefficients α and β which multiply neutron or proton spin densities $J_{(n\,\mathrm{or}\,p)}$ as explained, e.g., in Ref. [4]. This modification affects the single-particle spin-orbit potentials

$$U_{\mathrm{so}}^{(n\,\mathrm{or}\,p)} = \frac{W_0}{2r}\left(2\frac{d\rho_{(n\,\mathrm{or}\,p)}}{dr} + \frac{d\rho_{(p\,\mathrm{or}\,n)}}{dr}\right) + \left(\alpha\frac{J_{(n\,\mathrm{or}\,p)}}{r} + \beta\frac{J_{(p\,\mathrm{or}\,n)}}{r}\right), \tag{2}$$

especially in the case of spin-unsaturated subshells, which contribute significantly to the spin densities. One has

$$\alpha = \alpha_C + \alpha_T, \quad \beta = \beta_C + \beta_T, \tag{3}$$

where α_C, β_C come from the central, velocity-dependent part of the Skyrme force, whereas α_T, β_T come from the tensor component. Using the Skyrme force SLy5, the values of α_T and β_T were determined [4] to be $\alpha_T = -170$ MeV fm^5, $\beta_T = 100$ MeV fm^5, and we shall adopt these values.

In the nonrelativistic Skyrme-HF model, the radial HF equations can be expressed in terms of an energy-dependent equivalent potential V_{eq}^{lj}, that is,

$$\frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2}\psi(r) + \frac{l(l+1)}{r^2}\psi(r)\right] + V_{\mathrm{eq}}^{lj}(r,\epsilon)\psi(r) = \epsilon\psi(r), \tag{4}$$

where

$$V_{\mathrm{eq}}^{lj}(r,\epsilon) = \frac{m^*(r)}{m}U_0(r) + \frac{m^*(r)}{m}U_{\mathrm{so}}^{lj}(r) + V_{\mathrm{eq}}^{m*}. \tag{5}$$

Here, $U_{\mathrm{so}}^{lj}(r) = U_{\mathrm{so}}(r) \times [j(j+1) - l(l+1) - 3/4]$,

$$V_{\mathrm{eq}}^{m*} = \left[1 - \frac{m^*(r)}{m}\right]\epsilon - \frac{m^{*2}(r)}{2m\hbar^2}\left(\frac{\hbar^2}{2m^*(r)}\right)'^2 + \frac{m^*(r)}{2m}\left(\frac{\hbar^2}{2m^*(r)}\right)'', \tag{6}$$

and $U_0(r)$ and $m^*(r)$ are the HF central potential and effective mass, respectively [8]. The Coulomb potential is included in U_0, in the case of protons. With the help of Eqs. (4)–(6), we can write ϵ as a sum of kinetic, central, spin-orbit, and nonlocality (or m^*-dependent) contributions:

$$\epsilon = \epsilon_{\mathrm{kin}} + \epsilon_{\mathrm{cen.}} + \epsilon_{\mathrm{s.o.}} + \epsilon_{m*}. \tag{7}$$

In the above expression, the three last terms correspond to the three terms of Eq. (5). This decomposition is useful for understanding the evolution of single-particle energies when N or Z is changing [15], and it will be used in the discussion of results in Sec. III.

B. RHF-BCS mean field with density-dependent Lagrangians

Another type of mean-field approach is based on covariant effective Lagrangians. A very popular and successful version is the RMF (see, e.g., Ref. [16]). However, the RMF is only a Hartree approximation, and it cannot describe the effects of a two-body tensor interaction brought about by the exchange of pions or of ρ mesons with tensor coupling, because these effects would appear in the exchange (Fock) contributions to the total energy. Thus, the RMF approach is not suitable for our present purpose.

Recently, progress have been made with the RHF-BCS approach. New density-dependent effective Lagrangians have been proposed that are able to give a satisfactory overall description of bulk properties of nuclei throughout the mass table [9,17]. In this work, we will compare results obtained with two different effective Lagrangians: the parameter set PKO1 [9], which includes σ, ω, ρ vector and π exchanges, and the parameter set PKO2 [17], which does not include π exchange. Thus, comparing the predictions of PKO1 and PKO2 can give us an idea of the effects on single-particle spectra due to a tensor component in the interaction, since the Fock terms of the one-pion exchange are indeed sensitive to this tensor component.

The two effective Lagrangians PKO1 and PKO2 are treated in the RHF-BCS approximation within a spherical symmetry assumption as in the Skyrme HF-BCS case. The pairing interaction has the same functional form as in Eq. (1), and the interaction parameters $V_0^{(n\,\mathrm{or}\,p)}$ are adjusted as in the nonrelativistic case. The RHF-BCS equations are self-consistently solved in coordinate space [9,17].

III. RESULTS AND DISCUSSION

A. The $2s$-$1d$ proton spectra in $Z = 14$ isotopes

We first examine the evolution of the proton single-particle spectra of the $2s$-$1d$ shell in the isotopic chain $Z = 14$ when the neutron number increases from $N = 20$ (^{34}Si, $\nu 1f_{7/2}$ empty) to $N = 28$ (^{42}Si, $\nu 1f_{7/2}$ filled). The question of reduction of the proton $1d_{3/2}$-$1d_{5/2}$ spin-orbit splitting when going from ^{34}Si to ^{42}Si is particularly interesting. A shell model analysis of the data [3] found that this spin-orbit splitting is reduced by about 1.94 MeV if one fills the $1f_{7/2}$ neutron subshell.

In the left panel of Fig. 1, we present the $2s$-$1d$ proton levels calculated with the Skyrme force SLy5, with and without the tensor component of Ref. [4]. Corresponding results obtained with the RHF-BCS model are shown in the right panel, using the PKO1 (with pion exchange, i.e., with tensor coupling) and PKO2 (without pion exchange) parametrizations. The general downward trend of all results as a function of N is easily understood as an effect of the neutron-proton symmetry potential.

The calculated values of the proton spin-orbit splitting, $\Delta_{\mathrm{so}}(N) \equiv \epsilon_{1d_{3/2}} - \epsilon_{1d_{5/2}}|_N$ are shown in Table I. It can be seen that the reduction of $\Delta_{\mathrm{so}}(N)$ from $N = 20$ to 28 is practically zero for SLy5, but it becomes 1.52 MeV for SLy5+tensor. For PKO1 and PKO2 the reduction is 1.43 and 0.81 MeV, respectively. It seems that the tensor force helps reduce $\Delta_{\mathrm{so}}(N)$ in both the nonrelativistic and relativistic models.

Actually, the two relativistic models PKO1 and PKO2 differ not only by the pion-coupling term but also by the strengths of other meson-nucleon couplings; therefore, one cannot relate

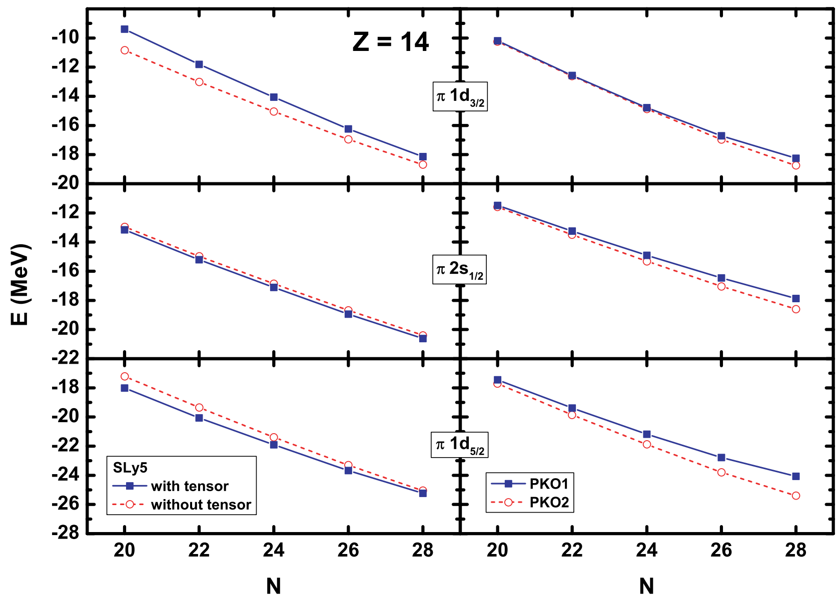

FIG. 1. (Color online) 2s-1d proton single-particle levels in the Si isotopic chain calculated in the mean-field approach. Left panel: nonrelativistic model with SLy5; right panel: relativistic model with PKO1 and PKO2.

the changes in $\Delta_{so}(N)$ only to the tensor coupling. On the other hand, it is an easier task to analyze the evolution of $\Delta_{so}(N)$ in the nonrelativistic model. We use the decomposition of Eq. (7) to cast $\Delta_{so}(N)$ into a sum of three terms: (1) a kinetic plus central contribution, (2) a spin-orbit contribution, and (3) a term due to $m^*(r) \leqslant m$ and related to the nonlocality of the mean field. These three terms are shown in Fig. 2. The kinetic and central contributions are of opposite signs and comparable magnitudes, their sum remains small from $N = 20$ to 28, and the tensor force has little effect on it. The spin-orbit term is nearly flat for SLy5, whereas the results of SLy5+tensor show a strong decrease of about 1 MeV. This effect is easily understood because of the properties of the Skyrme-HF mean field and of the neutron-proton tensor interaction. Firstly, the neutron spin density J_n becomes larger when one fills the neutron orbital $1f_{7/2}$ [8], then the proton spin-orbit potential which contains a term $\beta_T J_n$ decreases accordingly, since the contribution of $\beta_T J_n$ to the spin-orbit potential in Eq. (2) comes with a positive sign and thus it reduces the absolute value of the spin-orbit potential. The proton spin density remains the same for the entire chain, so the term $\alpha_T J_p$ contributes in a same way to all nuclei. Finally, the nonlocality term is flat for the SLy5 results but it decreases by about 300 keV from $N = 20$ to 28 for the SLy5+tensor case because it is practically proportional to $\Delta_{so}(N)$.

Thus it can be concluded that in the framework of the self-consistent mean field with Skyrme interactions, the reduction of the proton $1d_{3/2}$-$1d_{5/2}$ spin-orbit splitting in ^{42}Si can be attributed to the effect of a tensor component in the effective interaction. For the RHF-BCS model, one observes that the reduction is also enhanced by a tensor component brought about by a pion-induced interaction. However, all of the present discussion is done strictly in the framework of a static mean-field approach, and it must be kept in mind that

TABLE I. $1d_{3/2}$-$1d_{5/2}$ splitting for the nuclei $^{34-42}$Si calculated with the models described in the text; units are MeV.

(N, Z)	(20,14)	(22,14)	(24,14)	(26,14)	(28,14)
SLy5	6.38	6.33	6.35	6.35	6.36
SLy5+T	8.62	8.26	7.85	7.43	7.10
PKO1	7.26	6.81	6.41	6.07	5.83
PKO2	7.46	7.24	7.02	6.82	6.65

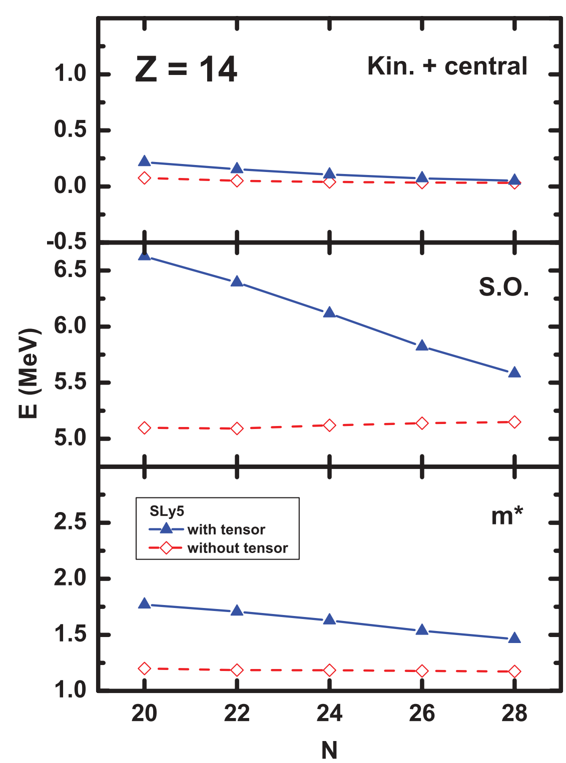

FIG. 2. (Color online) Contributions to $\Delta_{so}(N)$ according to the decomposition in Eq. (7). The results correspond to the Skyrme interaction SLy5, with (solid lines) and without (dashed lines) the tensor component.

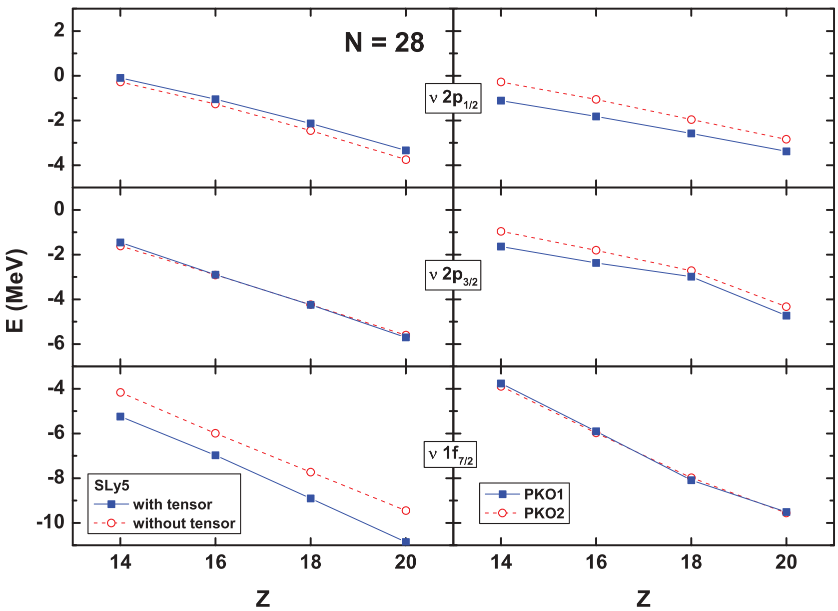

FIG. 3. (Color online) $2p_{1/2}, 2p_{3/2}$, and $1f_{7/2}$ neutron single-particle levels in the $N = 28$ isotonic chain calculated in the mean-field approach. Left panel: nonrelativistic model with SLy5; right panel: relativistic model with PKO1 and PKO2.

effects beyond mean field such as particle-vibration coupling [18] have to be evaluated for these nuclei. Because of these missing effects, one cannot compare directly our calculated spectra with empirical ones. Nevertheless, the predictions of the mean-field approach concerning evolutions of energy differences remain meaningful.

B. The $2p$-$1f$ neutron spectra in $N = 28$ isotones

We now discuss the changes of neutron single-particle energies in the $2p$-$1f$ shell when going along the $N = 28$ isotones from ^{48}Ca ($Z = 20$) to ^{42}Si ($Z = 14$).

Experimental observations combined with a shell model analysis [2,3] lead to the conclusion that a compression of the neutron $2p$-$1f$ spectrum occurs when one removes protons from the $1d_{3/2}$ and $2s_{1/2}$ orbitals, keeping $N = 28$ fixed. This compression could affect by about 1 MeV the distance between the neutron $1f_{7/2}$ and $2p_{3/2}$ states and reduce the $N = 28$ gap from 4.8 MeV in ^{48}Ca to about 3.8 MeV in ^{42}Si.

In Fig. 3, we present the energies of the three lowest states of the neutron $2p$-$1f$ shell calculated with the nonrelativistic and relativistic mean-field models. We observe again the downward trends as functions of Z, a manifestation of the increasing symmetry potential in the mean fields. Looking at the $N = 28$ gap, $\Delta_{\text{gap}}(Z) \equiv \epsilon_{2p_{3/2}} - \epsilon_{1f_{7/2}}|_Z$, we can see from Fig. 2 that in the nonrelativistic case, adding a tensor force affects little the $2p_{3/2}$ state but pulls down the $1f_{7/2}$ state and consequently increases $\Delta_{\text{gap}}(Z)$ for all Z values. On the other hand, in the relativistic case, the position of the $1f_{7/2}$ state is almost the same for both PKO1 and PKO2 parametrizations, but the $2p_{3/2}$ state is lower with PKO1 (with tensor component) than with PKO2, so the model with a tensor component seems to lead to smaller $\Delta_{\text{gap}}(Z)$. However, as noticed above, the differences between PKO1 and PKO2 are not only in the tensor component, unlike the case of SLy5 compared to SLy5+ tensor.

The calculated values of the $N = 28$ gap $\Delta_{\text{gap}}(Z)$ are displayed in Table II. It can be seen that all models predict a substantial reduction of this gap when going from $Z = 20$ (^{48}Ca) to $Z = 14$ (^{42}Si). The largest reduction is for the two models PKO1 (2.65 MeV) and PKO2 (2.29 MeV), whereas the Skyrme models SLy5 and SLy5+tensor predict a reduction of 1.20 and 1.36 MeV, respectively. These values are consistent with the experimental estimate of 1 MeV. The nonrelativistic results also indicate that the tensor component of the interaction does not play an essential role in this reduction. Although there are no numerical discrepancies, this conclusion is somewhat different from that of Ref. [7], mainly because in the latter case only two neighboring nuclei were studied, without the decomposition of Eq. (7). The present nonrelativistic result may be supported by the fact that both PKO1 and PKO2 relativistic models lead to very similar reduction.

One can have a closer look at the mechanism of this gap reduction by performing for the nonrelativistic models an analysis similar to that of Sec. III A. In Fig. 4 are shown the contributions to $\Delta_{\text{gap}}(Z)$ coming from the different terms of Eq. (7). Comparing the results of SLy5 and SLy5+tensor, one can see that the tensor force has an overall effect on the spin-orbit contribution to $\Delta_{\text{gap}}(Z)$, but it affects little the gap reduction from $Z = 20$ to $Z = 14$. The other two terms practically determine the gap reduction. In the SLy5+tensor case, for example, the partial decrease from $Z = 20$ to $Z = 14$ due to the kinetic+central effect is 840 keV, while the nonlocality effect is 564 keV.

TABLE II. $2p_{3/2}$-$1f_{7/2}$ gap for the isotonic chain $N = 28$; units are MeV.

(N, Z)	(28,14)	(28,16)	(28,18)	(28,20)
SLy5	2.55	3.09	3.49	3.75
SLy5+T	3.79	4.08	4.66	5.15
PKO1	2.13	3.52	5.11	4.78
PKO2	2.93	4.16	5.26	5.22

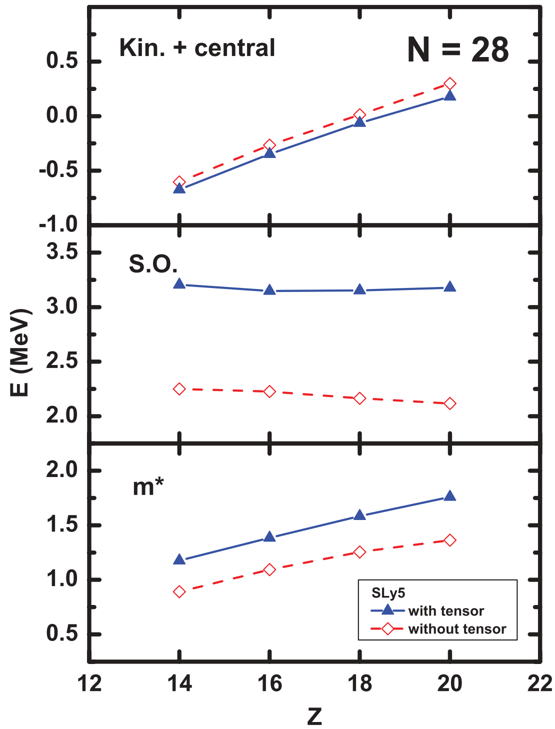

FIG. 4. (Color online) Three contributions to $\Delta_{\rm gap}(Z)$ according to the decomposition in Eq. (7). The results correspond to the Skyrme interaction SLy5, with (solid lines) and without (dashed lines) tensor component.

We stress again that in the present study, the particle-vibration effects are still missing, and their effects on $\Delta_{\rm gap}(Z)$ remain to be evaluated.

IV. CONCLUSION

In this work, we studied the mechanisms that lead to a reduction of the proton $1d_{3/2}$-$1d_{5/2}$ spin-orbit splitting $\Delta_{\rm so}(N)$ with decreasing mass number in the Si isotopic chain. We also investigated the quenching of the neutron $2p_{3/2}$-$1f_{7/2}$ gap $\Delta_{\rm gap}(Z)$ as one goes from ^{48}Ca toward ^{42}Si. We used the self-consistent mean-field approach in its nonrelativistic version with the SLy5 parametrization and its relativistic covariant version with exchange (Fock) terms.

One of the goals of this study was to determine to what extent a tensor component in the effective nucleon-nucleon interaction can affect the values of $\Delta_{\rm so}(N)$ and $\Delta_{\rm gap}(Z)$. Our main conclusions are (1) the reduction of $\Delta_{\rm so}(N)$ when going from ^{34}Si to ^{42}Si is mainly due to the presence of a tensor component in the effective interaction. The magnitude of the change in $\Delta_{\rm so}(N)$ is consistent with the empirical observations. (2) On the other hand, the evolution of $\Delta_{\rm gap}(Z)$ when Z decreases from 20 to 14 does not depend strongly on a tensor component in the interaction. These conclusions can be reached by using either a nonrelativistic Skyrme mean-field approach or a relativistic Hartree-Fock framework.

In the case of the Skyrme-Hartree-Fock model, we performed a detailed analysis of the origin of the evolution of $\Delta_{\rm gap}(Z)$ and $\Delta_{\rm so}(N)$. The reduction of the former can be traced back to changes occurring in the symmetry part of the central potential, to the m^* term of the Skyrme-HF model, and only to a small extent to the spin-orbit potential.

It would be important to extend in future studies this type of analysis to include effects such as particle-vibration coupling which are beyond the present mean-field models and which are known to affect single-particle spectra.

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