Systematic study of tensor effects in shell evolution

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In the framework of the Hartree-Fock-Bogoliubov approach with the Skyrme interactions SLy5, SLy5+T, SLy5+T$_w$, and several sets of the *TIJ* parametrizations (Skyrme effective interaction parametrizations including the tensor terms), the effect of the tensor force on the shell evolution at $Z, N = 8$, 20, and 28 is investigated. It is shown that the evolution of the gap (defined as the energy difference between the last occupied and first unoccupied single-particle orbits) with SLy5+T is similar to that with SLy5+T$_w$, and the gap values with SLy5+T are smaller than those with SLy5+T$_w$ in the cases of $Z, N = 8$, 20. At $Z, N = 28$, the gap values with SLy5 are smaller than those with SLy5+T and larger than those with SLy5+T$_w$. To understand these features, we analyze the spin-orbit potentials with and without the tensor contributions and the radial wave functions of relevant orbits. Meanwhile, we find that the deviation of the calculated gaps with SLy5+T$_w$ from the experimental ones is larger than that with SLy5+T. This indicates that SLy5+T$_w$ is not suitable for investigating the properties of the ground-state gap evolution. Finally, it is seen that the gap evolutions with different sets of the *TIJ* parametrizations are similar to each other except for the ones with T22, and there is almost no difference between the tensor effect in gap evolution with the perturbative method and the one with the complete fitting method.

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I. INTRODUCTION

The tensor force is an important and necessary ingredient of the nucleon-nucleon interaction [1,2], which has a crucial influence on the nuclear structure, such as the single-particle spectrum [3], nuclear matter with realistic potentials [4], deformation [5], and multipole giant resonances [6,7]. In the 1970s, some nuclear physicists pointed out that the tensor part of the nucleon-nucleon effective interaction has an important role in the spin-orbit splitting of the Hartree-Fock (HF) single-particle spectrum [8–12]. As a matter of fact, in the self-consistent mean-field theory, the effective zero-range nonlocal interaction proposed by Skyrme in 1956 contains a zero-range tensor force [13,14]. The first applications of the Skyrme interaction in self-consistent mean-field models that became available around 1970, however, neglected the tensor force, and the simplified effective Skyrme interaction used in the work by Vautherin and Brink [10] soon became the standard Skyrme interaction that has been used in most applications ever since. Until recent years, there has been only very little development of the Skyrme's tensor force. In the early work of Stancu *et al.* [3], they studied the tensor effects on the spin-orbit splitting of nuclei by adding the tensor force in a perturbative way in the 1970s. After that, most of the Skyrme forces were fitted without considering the contribution of the tensor part except for the work done by Tondeur and Liu *et al.* [15,16]. Recent studies indicate that the tensor force plays a crucial role in the evolution of shell structure in exotic nuclei based on the shell model [17–20]. Therefore, it is necessary to study the shell evolution and the modification of some magic numbers far from the stability in terms of the tensor effects in the framework of various self-consistent mean-field approaches, which is an interesting subject in nuclear structure study. Within mean-field models, for example, Skyrme-HF, the tensor force was usually added perturbatively into the existing standard parametrizations SIII and SLy5 in Refs. [21–23], respectively. In addition, the inclusion of the tensor force in the Skyrme-HF calculations achieved considerable success in explaining some features of the evolution of the single-particle states in medium mass nuclei.

Very recently, Torres *et al.* [24] discussed how the tensor component contributes to the evolution behavior of the proton (neutron) gaps at magic numbers $Z, N = 8$, 20, and 28 by using nonrelativistic Skyrme- and Gogny-HF models as well as relativistic Hartree-Fock (RHF) models and obtained some interesting results. It turned out that the tensor effects in the evolution of the magic gaps can be more easily identified in the cases of $Z, N = 8$ and 20. At $Z, N = 28$, the tensor effect was more complicated and mixed with other mean-field effects. However, the method they used neglected the pairing corrections, which is only suitable for investigating the closed-shell and assumed closed-shell nuclei. The main reason is that the GT2 parametrization that they adopted in the Gogny case has been fitted at the HF level. The use of this parametrization also in the pairing channel of a complete Gogny-HFB calculation could be questionable. Therefore, their obtained results can not reflect the gap evolution details in entire isotope and isotone chains. Then, it is interesting to study the properties of the gap evolution by taking into account the pairing corrections to study the gap evolution details. This constitutes the first motivation of this article. In addition, the tensor parametrizations obtained by the low-q

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limit of the G-matrix calculations in SLy5+T$_w$ are added perturbatively to the existing force SLy5. Note that the tensor part of SLy5+T$_w$ is different from that of SLy5+T, which was adopted in Ref. [21]. A recent study in Ref. [6] suggested that the charge exchange spin-dipole (SD) excitation of ^{208}Pb with SLy5+T$_w$ can better reproduce the experimental data than that with SLy5+T. Thus, it is necessary to investigate the properties of the ground-state shell evolution by using the SLy5+T$_w$ to test its validity. This is the second motivation. Recently, Lesinski *et al.* built a set of 36 Skyrme effective interaction parametrizations, including the tensor terms by a fitting method, which is called the *TIJ* parametrizations [25,26]. It is interesting to see the similarities and differences of the tensor effects on shell evolution due to use of the perturbative and complete fitting methods. This is the final motivation of this work. It is well known that the Skyrme parametrizations are suitable for investigating bulk properties of nuclei in the framework of the Hartree-Fock-Bogoliubov (HFB) theory [27–30], and with the pairing corrections taken into account by Bogoliubov transformation, the nuclear properties near drip lines can be better described than those with the BCS approximation. In addition, the viewpoint of Bogoliubov enhanced shell quenching was used to explain the abundance pattern from the astrophysical r process of nucleosynthesis [31,32]. Driven by the three motivations mentioned above, we investigate the gap evolutions at $Z, N = 8$, 20, and 28 isotope and isotone chains by using the HFB theory with Skyrme interactions SLy5, SLy+T, SLy5+T$_w$, and several sets of the *TIJ* parametrizations. This paper is organized as follows. In Sec. II, a theoretical framework is introduced. The numerical results and corresponding discussions are given in Sec. III. In the last section, the conclusions are drawn.

II. THEORETICAL FRAMEWORK

The tensor force has triplet-even and triple-odd zero-range terms, which read as

$$\begin{aligned}\upsilon_T = {} & \frac{T}{2}\left[(\sigma_1\cdot\mathbf{k}')(\sigma_2\cdot\mathbf{k}') - \frac{1}{3}(\sigma_1\cdot\sigma_2)\,\mathbf{k}'^2\right]\delta(\mathbf{r}_1-\mathbf{r}_2)\\ & + \frac{T}{2}\delta(\mathbf{r}_1-\mathbf{r}_2)\left[(\sigma_1\cdot\mathbf{k})(\sigma_2\cdot\mathbf{k}) - \frac{1}{3}(\sigma_1\cdot\sigma_2)\,\mathbf{k}^2\right]\\ & + U[(\sigma_1\cdot\mathbf{k}')\delta(\mathbf{r}_1-\mathbf{r}_2)(\sigma_2\cdot\mathbf{k})]\\ & - \frac{1}{3}U(\sigma_1\cdot\sigma_2)\times[\mathbf{k}'\cdot\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}], \end{aligned} \tag{1}$$

where $\mathbf{k} = (\nabla_1 - \nabla_2)/2i$ acts on the right, $\mathbf{k}' = -(\nabla_1 - \nabla_2)/2i$ on the left. T and U provide the intensity of the tensor force in even and odd states of relative motion, respectively. The tensor force and central exchange term lead to the contribution to the energy density as

$$\Delta H(\mathbf{r}) = \tfrac{1}{2}\alpha\left(J_n^2 + J_p^2\right) + \beta J_n J_p. \tag{2}$$

The spin-orbit potential is given by

$$U_{\text{s.o.}}^q = \frac{W_0}{2r}\left(2\frac{d\rho_q}{dr} + \frac{d\rho_{q'}}{dr}\right) + \left(\alpha\frac{J_q}{r} + \beta\frac{J_{q'}}{r}\right), \tag{3}$$

where $J_{q(q')}(\mathbf{r})$ is the proton or neutron spin-orbit density defined as

$$J_{q(q')}(r) = \frac{1}{4\pi r^3}\sum_i (2j_i+1) \times\left[j_i(j_i+1) - l_i(l_i+1) - \frac{3}{4}\right]R_i^2(r). \tag{4}$$

In this expression, q stands for neutrons (protons) and q' for protons (neutrons), where $i = n, l, j$ runs over all states having the given q (q'), and $R_i(r)$ is the radial part of the wave function.

The terms in the first parentheses of Eq. (3) come from the Skyrme spin-orbit interaction, and the terms in the second parentheses include both the central exchange and the tensor contributions. In Eqs. (2) and (3), $\alpha = \alpha_C + \alpha_T$, $\beta = \beta_C + \beta_T$. The central exchange contributions are written in terms of the usual Skyrme parameters as

$$\alpha_C = \tfrac{1}{8}(t_1 - t_2) - \tfrac{1}{8}(t_1x_1 + t_2x_2), \quad \beta_C = -\tfrac{1}{8}(t_1x_1 + t_2x_2). \tag{5}$$

Basic definitions of all quantities derived from the Skyrme parameters can be found in Refs. [10,13,14,30]. The tensor contributions are expressed as

$$\alpha_T = \tfrac{5}{12}U, \quad \beta_T = \tfrac{5}{24}(T + U). \tag{6}$$

With the definitions mentioned above, the spin-orbit potential can be written in the following form:

$$\begin{aligned} U_{\text{s.o.}}^q &= \frac{W_0}{2r}\left(2\frac{d\rho_q}{dr} + \frac{d\rho_{q'}}{dr}\right)\\ &\quad + \left(\alpha_C\frac{J_q}{r} + \alpha_T\frac{J_q}{r} + \beta_C\frac{J_{q'}}{r} + \beta_T\frac{J_{q'}}{r}\right)\\ &= \frac{W_0}{2r}\left(2\frac{d\rho_q}{dr} + \frac{d\rho_{q'}}{dr}\right)\\ &\quad + \left(\alpha_C\frac{J_q}{r} + \beta_C\frac{J_{q'}}{r}\right) + \left(\alpha_T\frac{J_q}{r} + \beta_T\frac{J_{q'}}{r}\right)\\ &= U_\rho + U_C + U_T. \end{aligned} \tag{7}$$

In this paper, all calculations were performed using the HFBRAD code [27] with the Skyrme force in the particle-hole channel. In the pairing channel, we use the mixing pairing interaction, which is written as

$$V = \left(t_0' + \frac{t_3'}{6}\rho^{\gamma'}\right)\delta, \tag{8}$$

where $t_3' = -18.75t_0'$, $\gamma' = 1$, and t_0' is an adjusted parameter which can be determined by the empirical pairing gaps. The pairing parameters corresponding to different versions of the Skyrme forces can be found in Table II of Ref. [27]. The box and mesh sizes are selected as 30 and 0.1 fm, respectively.

III. RESULTS AND DISCUSSIONS

We have performed systematic calculations for the gap evolution at $Z, N = 8$, 20, and 28 by using the HFBRAD code with the Skyrme interactions SLy5, SLy5+T, and SLy5+T$_w$. The theoretical results with and without the tensor force and

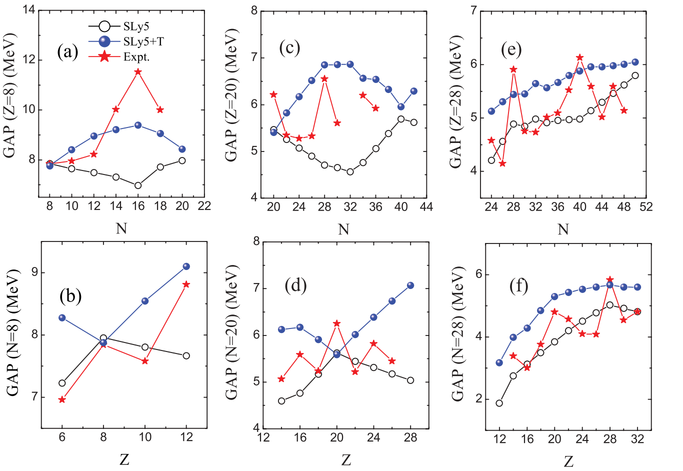

FIG. 1. (Color online) Comparison between the calculated gap evolutions at $Z, N = 8$, 20, and 28 with and without tensor force and experimental data. The Skyrme interaction with the tensor force is SLy5+T.

the available experimental data as functions of the proton number Z or neutron number N are plotted in Figs. 1 and 2. The gap is defined as the difference of the single-particle energies between the last occupied (below) orbit and the first unoccupied orbit (above). As to the values of experimental gaps, we can obtain them by using the approximate approach described in Ref. [24]. For the experimental gaps of the nuclei with $N = Z$, the Wigner correction is considered, which is the same as that in Refs. [24,33]. For the $Z, N = 8$ isotope and isotone chains, the gaps are specified by the energy difference of the first unoccupied proton (neutron) level $1d_{5/2}$ and the last occupied one $1p_{1/2}$. For the $Z, N = 20$ isotope and isotone chains, the gaps are measured by the energy difference of the proton (neutron) states $1f_{7/2}$ and $1d_{3/2}$. The gaps are determined by the energy difference of the proton (neutron) states $1f_{7/2}$ and $2p_{3/2}$ for the $Z, N = 28$ isotope and isotone chains.

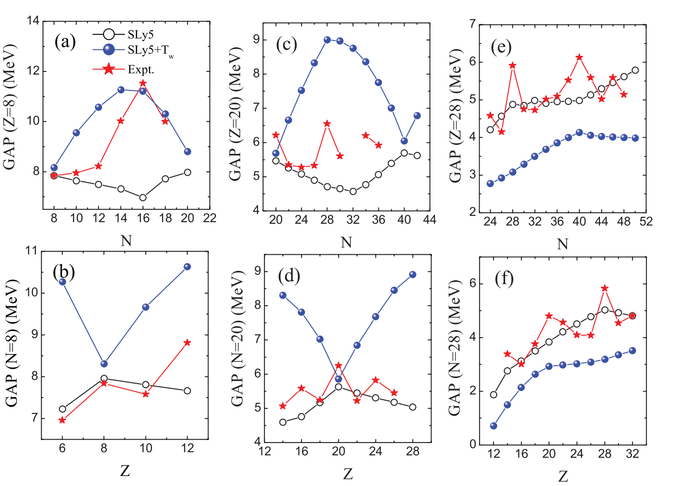

FIG. 2. (Color online) Same as Fig. 1, but the Skyrme interaction with the tensor force is SLy5+T$_w$.

From Figs. 1 and 2, we can see that the tensor force has almost no influence on the proton and neutron gaps for the nuclei ^{16}O and ^{40}Ca because they are the spin-saturated nuclei for both protons and neutrons. For ^{60}Ca, which is also a spin-saturated nucleus in the framework of the HF theory, the contribution of the tensor force to the gap almost vanishes. Nevertheless, a small gap change can be seen due to the presence of the pairing interaction. For other nuclei, the gaps are more strongly influenced by the tensor force. Concerning the gap evolution tendency with the tensor force, it can be described by the monopole effect proposed by Otsuka *et al.* [17–20]. However, our main concern is not the evolution tendency, but the similarities and differences of the gap evolutions with SLy5+T and SLy5+T$_w$. According to the comparisons between Figs. 1 and 2, it is not so difficult to find that there are the following interesting features:

(i) The gap evolutions varying with Z or N calculated with SLy5+T are similar to those with SLy5+T$_w$, and the gap values with SLy5+T are smaller than those with SLy5+T$_w$ for the cases of $Z, N = 8, 20$.
(ii) In the cases of $Z, N = 28$, the gap values with SLy5+T are larger than those with SLy5, whereas the gaps with SLy5+T$_w$ are smaller than those with SLy5.
(iii) Although all the calculated gaps with SLy5+T and SLy5+T$_w$ could not reproduce the experimental data well, the deviation of the calculated results with SLy5+T$_w$ from the experimental data is larger than that with SLy5+T.

We now discuss the first and the second features mentioned above by analyzing the spin-orbit potentials and the radial wave functions of selected orbits. The proton spin-orbit potentials and the radial wave function square of several selected proton orbits as functions of the radial distance r for ^{46,56}Ca and ^{68,78}Ni are plotted in Figs. 3, 4, 6, and 7, respectively.

From Fig. 3, one can see that the potential U_T with SLy5+T of ^{46,56}Ca is positive for all r. This is because Ca

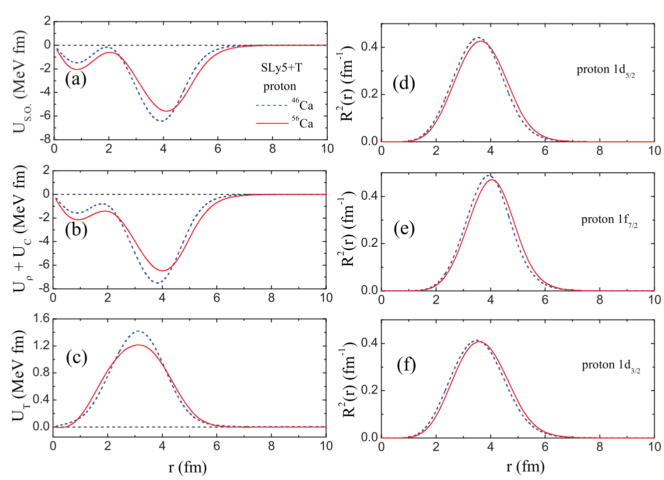

FIG. 3. (Color online) Proton spin-orbit potentials and the radial wave function square of the $1d_{5/2}$, $1f_{7/2}$, and $1d_{3/2}$ orbits in ^{46,56}Ca with SLy5+T.

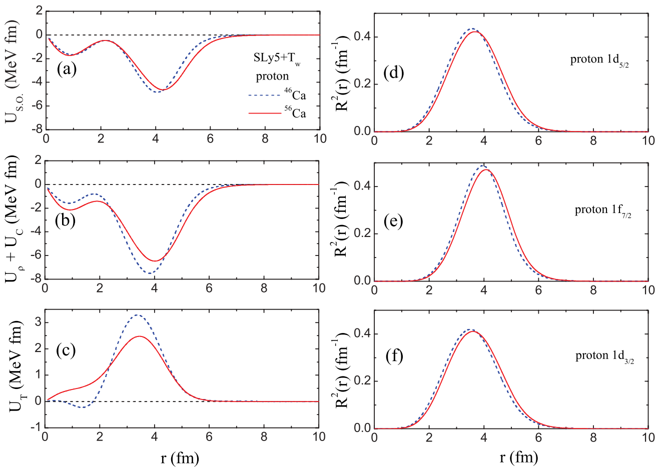

FIG. 4. (Color online) Same as Fig. 3, but the Skyrme interaction with the tensor force is SLy5+T$_w$.

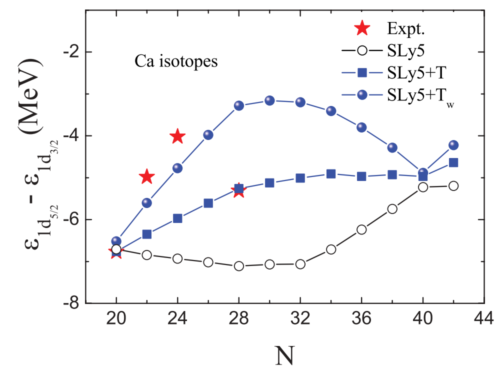

FIG. 5. (Color online) Energy differences between the $1d_{5/2}$ and $1d_{3/2}$ single proton states in Ca isotopes with the Skyrme interactions SLy5, SLy5+T, and SLy5+T$_w$.

isotopes are the spin-saturated nuclei for protons, and the tensor effect is practically attributable only to the filling of neutron orbits so that one gets no contribution from the proton spin current density J_p. In other words, U_T is only relevant to the parameter β_T and the neutron spin current density J_n. For SLy5+T, the neutron spin current density J_n and the β_T value ($\beta_T = 100$ MeV fm^5) are positive so that the tensor effect gives a positive contribution to U_T. For SLy5+T$_w$, the parameter β_T value takes to be 238.2 MeV fm^5. As a result, the potential U_T with SLy5+T$_w$ varying with r is similar to that of SLy5+T, and its values are larger than the ones in Fig. 3(c). These phenomena can be seen clearly according to the comparison between Figs. 3(c) and 4(c). Therefore, the first feature is explained by similar U_T with SLy5+T and SLy5+T$_w$. As to the wave functions, there are almost no differences between SLy5+T and SLy5+T$_w$. In addition, the wave functions of the $1d_{5/2}$, $1f_{7/2}$, and $1d_{3/2}$ orbitals and the total potential $U_{\text{s.o.}}$ are peaked around the same region. This suggests that these relevant orbits are strongly modified by the tensor contributions. In order to show this conclusion more evident, we also have made calculations on the proton single-particle energy differences between $1d_{5/2}$ and $1d_{3/2}$ orbitals in Ca isotopes with the Skyrme interactions SLy5, SLy5+T, and SLy5+T$_w$ and compared the calculated results with the experimental data, which are plotted in Fig. 5. The experimental points are taken from Ref. [34]. It is shown that the energy differences between $1d_{5/2}$ and $1d_{3/2}$ orbitals are influenced strongly by the tensor force, and the experimental data can be better reproduced by introducing the tensor force.

As seen from Fig. 6, the potential U_T with SLy5+T is changed a lot as the neutron number N varies from 40 to 50. This is because ^{68}Ni is a spin-saturated nucleus for neutrons so that U_T is only sensitive to the parameter α_T and the proton spin current density J_p. For SLy5+T, the potential U_T of ^{68}Ni is negative because of the positive J_p with the negative value of α_T ($\alpha_T = -170$ MeV fm^5). However, ^{78}Ni is a spin-unsaturated nucleus for protons and neutrons so that $U_T = \alpha_T \frac{J_p}{r} + \beta_T \frac{J_n}{r}$. Thus, the parameters α_T, β_T and the spin current densities J_n, J_p have contributions to U_T. One can get positive U_T from the second term. Therefore, the U_T value of ^{78}Ni moves up. For SLy5+T$_w$, the values of α_T and β_T are all positive ($\alpha_T = 134.76$ MeV fm^5, $\beta_T = 238.2$ MeV fm^5). Therefore, U_T becomes positive and its value is enhanced, which can be seen in Fig. 7(c) obviously. Hence, the second feature is explained by the opposite U_T with SLy5+T and SLy5+T$_w$. As to the wave functions, we can see clearly from Figs. 6 and 7 that each one has a slight change when the neutron number N goes from 40 to 50, and there is almost no difference between the results with SLy5+T and those with SLy5+T$_w$. Since the $2p_{3/2}$ orbit has nodes in the region between 3.5 and 4 fm, this orbit is not sensitive to the tensor force. Unlike the $1f_{5/2}$ and $1f_{7/2}$ orbitals, the two levels are strongly modified by the tensor force. In addition, because each wave function $R(r)$ is basically unchanged when N goes from 40 to 50, and the f shell splitting is reduced by the growing mismatch between the peaks of $R(r)$ and $U_{\text{s.o.}}$ when N goes from 40 to 50. This result is consistent with that of Otsuka *et al.* [19]. Just like their idea, this situation is different from the conventional explanation [35] that, in neutron-rich nuclei, the density decreases more slowly at the surface as a function of r, and thereby the magnitude of $U_{\text{s.o.}}$ becomes smaller, giving

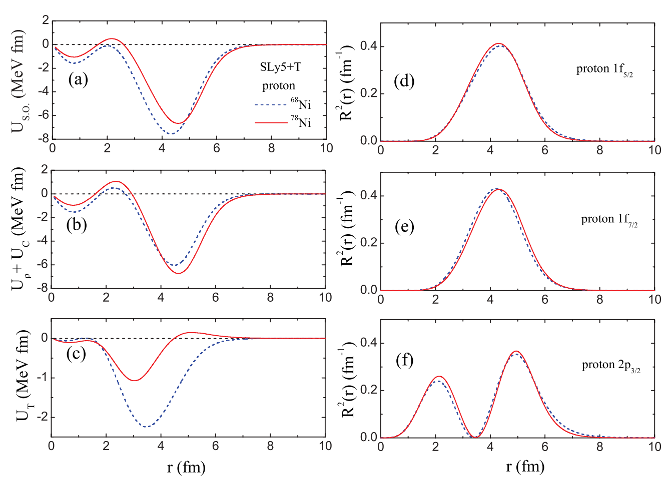

FIG. 6. (Color online) Proton spin-orbit potentials and the radial wave function square of the $1f_{5/2}$, $1f_{7/2}$, and $2p_{3/2}$ orbits in ^{68,78}Ni with SLy5+T.

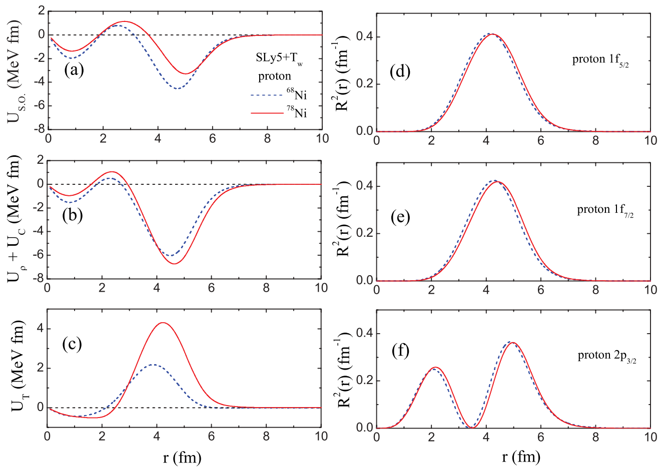

FIG. 7. (Color online) Same as Fig. 6, but the Skyrme interaction with the tensor force is SLy5+T$_w$.

rise to a reduced spin-orbit splitting. From the discussions in the previous paragraphs, we can clearly conclude that the shell evolution originates from the competition between the spin-orbit and tensor interactions.

It is well known that the tensor parametrizations in SLy5+T and SLy5+T$_w$ are all added perturbatively into the existing standard Skyrme parametrization SLy5. One recent work in Ref. [6] on the tensor force suggested that the charge exchange SD excitation of ^{208}Pb by using SLy5+T is larger than, and does not match, the experimental data. This indicates that SLy5+T$_w$ is better than SLy5+T in the study of excitation properties of nuclei. However, we obtain the opposite result according to the third feature, which indicates that the Skyrme parametrization with the tensor force SLy5+T$_w$ is not suitable for investigating the properties of the ground-state gap evolutions.

Recently, Lesinski and Bender *et al.* [25,26] built a set of 36 Skyrme effective interaction parametrizations (*TIJ* family), which cover a wide range of the parameter space of the isoscalar and isovector tensor coupling constants with a fit protocol very similar to that of the successful SLy parametrizations, and analyzed the impact of the tensor terms on a large variety of observables in spherical mean-field calculations [25]. In addition, we have noticed that the experimental data of the charge exchange SD excitation of ^{208}Pb can be well reproduced by the calculations in the framework of Hartree-Fock plus random phase approximation (HF+RPA) schemes with several sets of the *TIJ* parametrizations such as T22, T32, T43, and T44 [6]. Thus, it is interesting to study the tensor effects on the gap evolutions in the HFB model by using these *TIJ* parametrizations and, further, to see the similarities and differences between SLy5+T, SLy5+T$_w$, and the *TIJ* effective interaction parametrizations. The calculated gap evolutions at $Z, N = 8$, 20, and 28 with these *TIJ* parametrizations are shown in Fig. 8. One can see that the gap evolutions with these *TIJ* parametrizations are similar to each other except for the ones with T22. This is because the sum of U_C and U_T terms will have no contributions to the spin-orbit potential $U_{\text{s.o.}}$ at sphericity when the tensor force is taken into account ($\alpha = 0$, $\beta = 0$). In other words, the gap evolutions with T22 are not sensitive to the filling of proton or neutron orbitals. In addition, according to the comparisons between the calculated results in Fig. 8 and those in Figs. 1 and 2, it is not difficult to find that there are almost no differences between the gap evolutions with SLy5+T, SLy5+T$_w$, and those with the *TIJ* parametrizations. However, this conclusion needs to be further tested by future calculations.

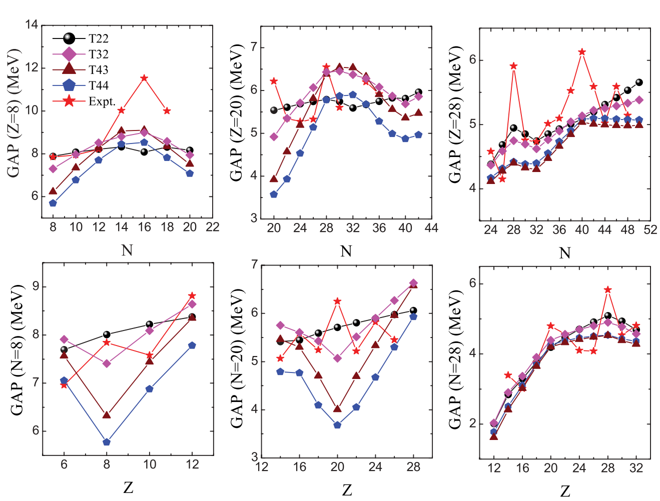

FIG. 8. (Color online) Gap evolutions at $Z, N = 8$, 20, and 28 with Skyrme interactions T22, T32, T43, and T44.

IV. CONCLUSIONS

In this paper, the tensor effects on gap evolutions at $Z, N = 8$, 20, and 28 have been investigated with the Skyrme interactions SLy5, SLy5+T, SLy5+T$_w$, and several sets of the *TIJ* parametrizations in the framework of the HFB approach. According to the comparisons of the calculated results with SLy5+T and SLy5+T$_w$, we find that the gap evolutions with SLy5+T varying with Z or N are similar to those with SLy5+T$_w$ and the gap values with SLy5+T are smaller than those with SLy5+T$_w$ for the cases of $Z, N = 8, 20$. In the cases of $Z, N = 28$, the gap values with SLy5+T are larger than those with SLy5, whereas the gaps with SLy5+T$_w$ are smaller than those with SLy5. For these features, we have attributed them to the competition between the spin-orbit and the tensor interactions. In addition, we also find that the deviation of the calculated gaps with SLy5+T$_w$ from the experimental data is larger than that with SLy5+T. This indicates that SLy5+T$_w$ is not suitable for investigating the properties of the ground-state gap evolutions, although it can reproduce the experimental data of the charge exchange SD excitation. At last, it is necessary to point out that one can get similar gap evolutions with different sets of the *TIJ* parametrizations except for T22, and there are almost no differences between the calculated results with the perturbative method and those with the complete fitting method. Because we just make calculations by using a limited number of the *TIJ* parametrizations, the conclusion needs to be further tested by more calculations.

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