Evolution of nuclear shell structure due to the pion exchange potential

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Abstract – The evolution of nuclear shell structure is investigated for the first time within density-dependent relativistic Hartree-Fock theory and the role of $\pi$-exchange potential is studied in detail. The energy differences between the neutron orbits \{$\nu_1h_{9/2}, \nu_1i_{13/2}$\} in the $N=82$ isotones and between the proton ones \{$\pi_1g_{7/2}, \pi_1h_{11/2}$\} in the $Z=50$ isotopes are extracted as a function of neutron excess $N-Z$. A kink around $Z=58$ for the $N=82$ isotones is found as an effect of pion correlations. It is shown that the inclusion of $\pi$-coupling plays a central role to provide substantial isospin dependence of the energy differences. In particular, the tensor part of the $\pi$-coupling has an important effect on the characteristic isospin dependence observed in recent experiments.

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The nucleon-nucleon bare interaction at low and medium energies is originally induced by the meson exchange processes as predicted by Yukawa [1]. In the nuclear medium, it is strongly renormalized by medium effects which lead to the effective nucleon-nucleon interaction. A large part of the present understanding of nuclear structure is based on self-consistent mean-field descriptions making use of effective interactions directly parametrized so as to reproduce selected nuclear properties. The two most successful categories are the non-relativistic Hartree-Fock approaches [2–5] and the relativistic mean-field (RMF) approaches [6–8]. Using these models, many nuclear-structure properties are calculated in the whole region of the nuclear chart with density-dependent effective interactions [9–23]. During the past decade, great successes have been achieved by the RMF theory not only in stable nuclei but also in exotic regions [18–26]. Of special interest is the fact that the RMF model provides a natural mechanism for explaining the spin-orbit splittings of single-particle levels. This feature becomes even more of central importance with the experimental observation that nuclei near drip lines undergo modifications of their shell structure, where the spin-orbit potential must play an essential role.

One of the basic open problems is the role of the one-pion exchange process, which is known to play a fundamental role in the meson-exchange interaction. However, the RMF model is not the appropriate framework to study pion-related processes because it is essentially a Hartree approximation where the Fock (exchange) contributions are altogether dropped, while the Hartree (direct) contributions of pions are zero due to the parity conservation in spherical and axially deformed nuclei. Recent progress in the relativistic Hartree-Fock description of nuclear structure, namely the density-dependent relativistic Hartree-Fock (DDRHF) theory [27] has brought a new insight to consider this problem. Within the DDRHF theory, the effective meson-nucleon coupling strengths including the one-pion exchange are determined in a similar way to the RMF model and a quantitative description of the nuclear-structure properties can be successfully achieved [27–29]. Thus, DDRHF
opens the possibility to investigate the role of one-pion exchange processes in nuclear-structure problems within the framework of a relativistic mean-field theory.

In this work, we study the role of pion-exchange processes on single-particle spectra by concentrating on specific cases. In the recent paper of Schiffer et al. [30], it was shown that a set of states outside the proton core $Z = 50$ and the neutron core $N = 82$ may provide a unique information to determine the evolution of the nuclear shell structure. This is why we choose here to discuss the pion effects taking these nuclei as an illustrative example.

The one-pion exchange process with pseudo-vector coupling contains two types of contributions, the central coupling and the non-central tensor coupling [31]. Recently, the tensor-type force was shown to have a distinct effect on the evolution of the nuclear shell structure in non-relativistic Hartree-Fock models [32,33].

In this work, we will study the behavior of single-particle energies of the states \( \{\nu l_{9/2}, \nu l_{13/2}\} \) (\( \nu \) denotes neutron states) in the \( N = 82 \) isotones and the states \( \{\pi l_{7/2}, \pi h_{11/2}\} \) (\( \pi \) denotes the proton states) in the \( Z = 50 \) isotopes within the DDRHF theory. The effect of the \( \pi \)-coupling, especially the contribution of its tensor component on the isospin dependence of the shell evolution will be analyzed in detail.

In a non-relativistic reduction, the one-pion exchange potential can be divided into two parts, \( V_\pi^c(q) \) and \( V_\pi^T(q) \):

\[
V_\pi^c(q) = -\frac{1}{3} \left[ \frac{f_\pi}{m_\pi} \right]^2 \frac{\sigma_1 \cdot \sigma_2 q^2}{m_\pi^2 + q^2} \vec{r}_1 \cdot \vec{r}_2, 
\]

(1a)

\[
V_\pi^T(q) = -\frac{1}{3} \left[ \frac{f_\pi}{m_\pi} \right]^2 \frac{3 \sigma_1 \cdot q \sigma_2 \cdot q - \sigma_1 \cdot \sigma_2 q^2}{m_\pi^2 + q^2} \vec{r}_1 \cdot \vec{r}_2. 
\]

(1b)

The Fourier-transform of the central part gives a repulsive contact interaction and an attractive Yukawa potential,

\[
V_\pi^c(r) = -\frac{m_\pi^3}{12\pi} \left[ \frac{f_\pi}{m_\pi} \right]^2 \sigma_1 \cdot \sigma_2 \left[ \frac{4\pi}{m_\pi^2} \delta(r) - \frac{e^{-m_\pi r}}{m_\pi r} \right] \vec{r}_1 \cdot \vec{r}_2.
\]

(2)

In general, the repulsive contact part is strongly hindered by the Pauli principle between two nucleons. Moreover, in DDRHF the \( \omega \)-meson exchange will strongly suppress the repulsive contact part so that it can be discarded on a solid basis [27]. The central part of the \( \pi \)-induced potential is thus given by

\[
V_\pi = \frac{1}{2} \sum_{\alpha \beta \gamma \delta} c_\alpha c_\beta c_\gamma c_\delta \int dr_1 dr_2 f_\alpha(r_1) f_\beta(r_2) \times \left[ \Gamma_\pi^e v_\pi \right]_{(1,2)} f_\gamma(r_2) f_\delta(r_1),
\]

(3)

where \( c_i \) and \( c_i^\dagger \) correspond to nucleon annihilation and creation operators, and the interaction vertex including the propagator is

\[
\left[ \Gamma_\pi^e v_\pi \right]_{(1,2)} = \vec{r}_1 \cdot \vec{r}_2 \left[ f_\pi \gamma \gamma_5 \right]_1 \cdot \left[ f_\pi \gamma \gamma_5 \right]_2 \frac{e^{-m_\pi |r_1 - r_2|}}{12\pi |r_1 - r_2|}. 
\]

(4)

Table 1: The effective interactions of DDRHF: PKO1, PKO2 and PKO3. The masses (in MeV) of nucleon, \( \omega \)-, \( \rho \)- and \( \pi \)-mesons are, respectively, taken as \( M = 938.9, m_\omega = 783.0, m_\rho = 769.0 \) and \( m_\pi = 138.0 \).

| PKO1 | PKO2 | PKO3 | PKO1 | PKO2 | PKO3 |
|------|------|------|------|------|------|
| \( m_\sigma \) | 525.77 | 534.46 | 525.67 | \( a_\sigma \) | 1.3845 | 1.3758 | 1.2446 |
| \( g_\sigma \) | 8.8332 | 8.9206 | 8.8956 | \( b_\sigma \) | 1.5132 | 2.0644 | 1.5667 |
| \( g_\omega \) | 10.7301 | 10.5510 | 10.8030 | \( c_\sigma \) | 2.2966 | 3.0524 | 2.0746 |
| \( g_\rho \) | 2.6290 | 4.0683 | 3.8325 | \( d_\rho \) | 0.3810 | 0.3305 | 0.4008 |
| \( f_\pi \) | 1.0000 | -1.0000 | 1.0000 | \( a_\omega \) | 1.4033 | 1.4514 | 1.2457 |
| \( a_\rho \) | 0.0768 | 0.6316 | 0.6353 | \( b_\omega \) | 2.0087 | 3.5744 | 1.6458 |
| \( a_\pi \) | 1.2320 | -0.9341 | 1.2341 | \( c_\omega \) | 3.0467 | 5.4784 | 2.1771 |
| \( \rho_\sigma \) | 0.1520 | 0.1510 | 0.1530 | \( d_\pi \) | 0.3308 | 0.2467 | 0.3913 |

The tensor \( \pi \)-coupling \( V_\pi^T \) can be obtained by subtracting the central part from the total \( \pi \) contributions.

In this work, the DDRHF calculations are performed with 3 parameter sets introduced in refs. [27,28]. They are denoted by PKO1, PKO2, PKO3, and their parameters are given in table 1. The DDRHF results are compared with RMF (Hartree) results calculated with the parameter set PKDD [23]. The effective interactions used here can provide appropriate quantitative descriptions of the properties of finite nuclei including binding energies, radii and spin-orbit splittings. It should be noticed that PKO3 has a stronger \( \pi \)-coupling than PKO1, while PKO2 and PKO3 have no \( \pi \)-coupling in the Lagrangian. The nuclei studied are located around the isotones with \( N = 82 \) from \( ^{132}\text{Sn} \) to \( ^{156}\text{W} \) and the Sn isotopes with \( Z = 50 \) from \( ^{104}\text{Sn} \) to \( ^{134}\text{Sn} \). For these open-shell nuclei, the pairing correlations are treated by the BCS method with a density-dependent, zero-range pairing force [34],

\[
V(r_1, r_2) = V_0 \delta(r_1 - r_2) \left[ 1 - \frac{\rho_0(r)}{\rho_0} \right],
\]

(5)

where \( V_0 = -850 \text{MeV} \cdot \text{fm}^3 \). The active pairing space is limited to the single-particle states below the single-particle energy +5 MeV. For the studied nuclei, the pairing correlations have minor effects in determining the shell structures and their evolutions.

The energy differences \( \Delta E(Z) \) between two unoccupied neutron states \( \{\nu l_{9/2}, \nu l_{13/2}\} \) of the \( N = 82 \) isotones are shown in the first panel of fig. 1 while the values \( \Delta E(N) \) between two unoccupied proton states \( \{\pi l_{7/2}, \pi h_{11/2}\} \) of the \( Z = 50 \) isotopes are shown in the second panel. The results of pion-dependent models PKO1 and PKD3 show kinks at \( Z = 58 \) \( (N = Z = 24, \text{i.e.,} \, ^{110}\text{Ct}) \) for the \( N = 82 \) isotones. In contrast, the pion-independent models PKO2 and PKDD predict a monotonous decrease with respect to \( N - Z \). A similar isospin dependence is also observed for the proton states of the Sn isotopes in the second panel of fig. 1: the inclusion of \( \pi \)-coupling in RHF (PKO1 and PKO3) brings an appreciable improvement compared with the results calculated without \( \pi \)-coupling (PKO2 and
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Fig. 1: (Color online) The energy differences $\Delta E(Z) = E_{\nu_{1\hbar_9/2}} - E_{\nu_{1\hbar_9/2}}$ in $N = 82$ isotones (first panel), and $\Delta E(N) = E_{\pi_{1h_{11/2}}} - E_{\pi_{1g_{7/2}}}$ in $Z = 50$ isotopes (second panel) as a function of neutron excess. The DDRHF results are due to PKO1, PKO2, PKO3, while the RMF results are obtained with PKDD. The experimental data are extracted from ref. [30].

PKDD). Around $^{112}$Sn there exists a small kink in the data and only PKO3 gives such a trend, which might be due to its stronger $\pi$-coupling than that of PKO1.

For the experimental data as shown in fig. 1, both kinks are located around the number 64 for protons or neutrons, corresponding to the so-called sub-shell closure. A common disease of RMF and RHF approaches is that the proton sub-shell at $Z = 64$ cannot be well reproduced and an artificial sub-shell closure at $Z = 58$ is found in both models [35]. This is the reason why PKO1 and PKO3 show kinks at $Z = 58$ instead of $Z = 64$ in the $N = 82$ isotones. In the middle of the shell, the single-particle states generally spread over some energy range due to configuration mixing. Recently, the fragmentation and spreading of the single-particle strength of the $1_{h_{11/2}}$ proton state in $^{114}$Sn has been studied in ref. [36] and it was found that this effect increases the $\Delta E = E_{\nu_{1h_{11/2}}} - E_{\nu_{1g_{7/2}}}$ by about 500 keV, while the effect is small in the doubly closed-shell nucleus $^{132}$Sn. Since the origin of the energy scale in fig. 1 (lower panel) is at $^{114}$Sn, the empirical point at $N = Z = 32$ should go down by 500 keV.

Fig. 2: (Color online) Central and tensor pion contributions to the energy differences $\Delta E(Z) = E_{\nu_{1\hbar_9/2}} - E_{\nu_{1\hbar_9/2}}$ in $N = 82$ isotones (first panel), and $\Delta E(N) = E_{\pi_{1h_{11/2}}} - E_{\pi_{1g_{7/2}}}$ in $Z = 50$ isotopes (second panel) as a function of neutron excess. The results are calculated by DDRHF with PKO1.

Taking into account this spreading effect when comparing mean-field predictions and data would bring the results of $\Delta E = E_{\pi_{1h_{11/2}}} - E_{\pi_{1g_{7/2}}}$ calculated with PKO1 or PKO3 in better agreement with experiment.

The single-particle energies contain contributions from the different mesons. The pion contributions can in turn be separated into a central and a tensor component. In fig. 2 are shown the $\pi$-coupling contributions to the $\Delta E(Z)$ in the $N = 82$ isotones and the $Z = 50$ isotopes calculated with PKO1. Comparing to the first panel of fig. 1, one can see that the characteristic isospin dependence of $\Delta E$, namely the kink at $Z = 58$, is mainly due to the pion coupling and particularly to its tensor part. For the $Z = 50$ isotopes, the kink cannot be reproduced by DDRHF with PKO1. In the second panel it is shown that the pion coupling, in fact its tensor part, reproduces this characteristic isospin dependence very well. In addition, one can also find another kink at the magic number $N = 82$, which reflects the shell effects as discussed above.

Let us now examine the configuration dependence of the $\pi$-coupling contributions. From $^{132}$Sn to $^{156}$W the added protons will gradually occupy the valence orbits $\pi_{1g_{7/2}}, \pi_{2d_{5/2}}, \pi_{2d_{3/2}}$ and $\pi_{1h_{11/2}}$. In fig. 3 we separate

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the contributions of $\pi$-coupling to $\Delta E(Z)$ into three components from the neutron core orbits ($N = 82$), the proton core orbits ($Z = 50$) and the valence proton orbits, respectively. From the first panel of fig. 3, it is seen that the valence protons play the most important role to give the isospin dependence shown in fig. 1 and fig. 2. In the second panel of fig. 3, the contributions of 4 valence proton orbits to $\Delta E(Z)$ are separately plotted to examine the configuration dependence of the tensor $\pi$-coupling. As the proton number increases from $Z = 50$ to 64 ($N - Z = 32$ to 24), the $\pi g_{7/2}$ orbit is gradually occupied. Then, from $Z = 60$ to 64 ($N - Z = 22$ to 18), the protons fill the $\pi d_{5/2}$ orbit and finally the $\pi h_{11/2}$ orbit is populated in the nuclei with $Z = 66 - 74$ ($N - Z = 16$ to 8). It is found from the second panel of fig. 3 that the magnitude of the tensor correlation is very sensitive to the occupation probabilities of the valence orbits, especially, those of high-$j$ orbits. Due to the existence of the artificial shell closure $Z = 58$ between the states $\pi g_{7/2}$ and $\pi d_{5/2}$, the valence protons can only sequentially fill the orbitals instead of spreading over these two orbits when the proton number increases from $Z = 50$ to 64. This also partially explains the reason of the discrepancy between the theoretical calculations and the experimental data.

In order to clarify the contributions of these valence proton states, we calculate the interaction matrix elements of $\pi$-coupling, separating the central and tensor parts, $V_{ab}^{C(C)}$ and $V_{ab}^{T}$. Figure 4 shows the central (first panel) and tensor (second panel) matrix elements between the neutron states ($\nu h_{9/2}$ (filled symbols) and $\nu l_{13/2}$ (open symbols)) and valence proton states ($\pi g_{7/2}$ (squares), $\pi d_{5/2}$ (circles), $\pi d_{3/2}$ (up-triangles) and $\pi h_{11/2}$ (down-triangles)) induced by the $\pi$-coupling as function of $N - Z$ in the $N = 82$ isotones. The results correspond to DDRHF with PKO1.

The first panel of fig. 4 shows that the central $\pi$-coupling is always attractive. As a result, it provides the simple monotonous behavior and weak isospin dependence (see fig. 2). At first sight, the tensor $\pi$-coupling
looks more complicated. However, one can find the following regularities: 1) the isospin dependence of the matrix elements is determined by the occupation probabilities of the valence proton orbits. 2) The tensor \(\pi\)-coupling is attractive for \((j_c,j_o)\) configurations, while it is repulsive for \((j_o,j_c)\) and \((j_c,j_o)\) configurations. 3) The magnitude of the tensor interaction matrix element is proportional to the degeneracy \(2j+1\) of the orbit. This peculiar feature of the tensor interaction was already pointed out in the deuteron binding mechanism in ref. [37], and also in the non-relativistic HF calculations [32,33]. These properties of the tensor force in DDRHF with PKO1 and PKO3 guarantee the isospin dependence of the energy difference between \(\nu l_{9/2}\) and \(\nu l_{11/2}\) to be consistent with the shell closure \(Z=58\), although it is artificial. In the Sn region, one can also find a similar consistency for the isospin dependence of the energy difference between \(\pi l_{9/2}\) and \(\pi l_{11/2}\) (see the second panels of fig. 1 and fig. 2).

In this work, the evolutions of nuclear shell structure outside the \(N=82\) neutron and \(Z=50\) proton closed shells are investigated for the first time within the density-dependent relativistic Hartree-Fock (DDRHF) theory and the role of the one pion-exchange potential is studied in detail. The energy differences \(\Delta E(N-Z)\) between the states \(\nu l_{9/2}, \nu l_{13/2}\) in the \(N=82\) isotones, and those between \(\pi l_{9/2}, \pi l_{11/2}\) in the \(Z=50\) isotopes are extracted as a function of neutron excess to explore the shell evolution of these exotic nuclei. It is found that the isospin dependence of \(\Delta E(N-Z)\) is consistent with the shell structure evolution if one includes a pion coupling term in the effective Lagrangian. This pion coupling gives the characteristic isospin dependence observed in recent experiments. Furthermore, the tensor \(\pi\)-coupling with the valence protons provides the important physical mechanism to give a proper description of the isospin dependence. Indeed, the strong configuration dependence of the tensor part of the \(\pi\)-coupling plays a crucial role to give the kink of the \(\Delta E(N-Z)\) observed in the experimental systematics of the shell evolution. It is also found that the appropriate description of the shell structure is very essential to reproduce the data.

Compared with the experimental results, however, there still exist some substantial discrepancies. Since the single-particle states studied in the present work are unoccupied orbits, the dynamical coupling to the core vibrations which is not considered here, might be one missing physical mechanism to cure the existing disagreement. In the present DDRHF the \(\pi\)-nucleon effective coupling, determined by fitting the empirical data of the ground-state properties of selected nuclei, is density dependent and its strength turns out to be fairly weak in the medium [28]. Another promising meson coupling for the shell evolution is the Lorentz \(\rho\)-tensor coupling which is not included yet. As a perspective, the inclusion of dynamical coupling to core vibrations, and of \(\rho\)-tensor coupling may play an additional important role to cure the existing discrepancies, especially for the artificial shell closures.

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