Nuclear structure around ^{80}Zr*

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Abstract Recent years have witnessed intense activity concerning the study of nuclei with equal numbers of neutrons and protons ($N = Z$). Exotic properties have been exhibited in the $N = Z$ nuclei, especially in those with atomic masses around 80. In the present paper, the projected shell model (PSM) together with a relativistic Hartree-Bogoliubov (RHB) theory is used to study the nuclear structure near the $N = Z$ line in the mass $A \approx 80$ region. For three Zr isotopes ^{80,82,84}Zr, the projected potential energy surfaces and ground state bands are calculated. It is shown that shape coexistence occurs in all of these nuclei. Moreover, we find that the residual neutron-proton interaction strongly affects the ground state band of ^{80}Zr; however, it slightly modifies those of ^{82}Zr and ^{84}Zr.

Key words projected shell model, relativistic Hartree-Bogoliubov theory, potential energy surface, ground state band, residual neutron-proton interaction

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1 Introduction

There has been longstanding interest in the structure of medium mass $N = Z$ nuclei since the $N = Z$ proton-rich nuclei with mass numbers around 80 exhibited phenomena that are unique to this mass region. Unlike the mid-rare earths and actinides that have very stable deformations, the structure of the neighboring nuclei in the mass $A \approx 80$ region changes abruptly. Moreover, this mass region is often characterized by shape coexistence. The study of these proton-rich nuclei is not only interesting from the nuclear structure point of view, it also has important implications in nuclear astrophysics. Nuclei of particular interest to the rp process are the $N = Z$ waiting-point nuclei. It has been argued that the existence of isomers in nuclei along the rp process path could significantly modify the current conclusions on nucleosynthesis and correlated energy generation in X ray bursts [1].

For $N = Z$ nuclei, there is currently an open question: whether the neutron-proton (n-p) correlation plays an important role in their structure. Recent experiments [2–4] have demonstrated that the rotational alignment for the $N = Z$ nuclei in the mass $A \approx 80$ region is considerably delayed compared with their neighboring nuclei. Sun et al. [5] investigated whether this observation can be understood by a known component of nuclear residual interactions in the projected shell model (PSM) approach. It was presented that the n-p quadrupole-quadrupole interaction, which is conjectured to be relevant for $N = Z$ nuclei, is shown to be quite important in explaining the delayed alignment. War et al. [6] made an attempt to study the effects of inclusion of n-p pairing in the $A = 68$–88, $N = Z$ nuclei in the framework of the variation-after-projection (VAP) technique. They included the pairing effects for both like particles as well as neutrons and protons. According to their calculations [6], the following conclusion was drawn: the

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yrast spectra based on the Hartree-Bogoliubov (HB) calculations clearly indicate that it is very important to include the n-p pairing effects for the structure of the $N=Z$ nuclei.

As we know, ^{80}Zr is one of the typically exotic nuclides in the mass $A \approx 80$ region. For ^{80}Zr, the subshell gap ($N = Z = 40$) is very large. Neutrons and protons are mainly distributed in the pf-shell and all the pf orbitals are filled. At the deformed potential minimum, the high-j $g_{9/2}$ orbitals intrude into the pf-shell near the Fermi level. A series of unique phenomena, including shape coexistence, may appear in ^{80}Zr. Nevertheless, the most important problem is whether the n-p pairing correlations affect the structure of the $N=Z$ nuclei ^{80}Zr. Thus it is interesting and significant to study the structure around ^{80}Zr.

The ground state band of ^{80}Zr has been observed only up to spin $I^{\pi}=10^{+}$ effectively due to low cross-sections, and shows evidence for a delayed alignment [2, 3] compared with its adjacent nuclei. This delay might be a signature for n-p pairing correlations. As mentioned above, Sun et al. [5] gave a satisfactory interpretation for the delay in the $N=Z$ nuclei such as ^{72}Kr and ^{76}Sr by increasing the n-p quadrupole-quadrupole interaction in the PSM approach. The PSM has actually become a standard tool to study the structure of deformed nuclei. Not long ago, the angular-momentum projected potential energy surface (PES) was carried out by means of the PSM approach to calculate the shapes of the deformed nuclei [7,8]. The PES naturally serves as a powerful tool to study nuclear shape coexistence and shape phase transitions [7].

In this paper, we will study the nuclear structure of ^{80}Zr. For comparison, the structure of its adjacent nuclei ^{82}Zr and ^{84}Zr will also be investigated. We will determine the quadrupole deformations of the ground state bands of the three Zr isotopes (^{80,82,84}Zr) by calculating the projected PES which is based on the PSM combined with a relativistic Hartree-Bogoliubov (RHB) theory. Then the ground state bands of these nuclei will be calculated by applying the PSM approach and comparing with the experimental data. Certainly, the residual n-p interaction will be carefully considered in our calculations.

2 The projected shell model and method of calculation of potential energy surfaces

The PSM [9–13] is a spherical shell model truncated in a deformed basis, which is a microscopic theory and solves the many-nucleon system fully quantum mechanically. The PSM proceeds as follows: The truncation is firstly done in the multi-quasiparticle (multi-qp) basis by selecting low-lying states; then the rotational symmetry (and the number conservation, if necessary) is restored for these (multi-qp) states by the projection method to form a spherical (many-body) basis in the laboratory frame; finally, the Hamiltonian is diagonalized in this basis.

We would recapitulate the most relevant points of the PSM calculations which will be used in the rest of this paper. The ansatz for the angular-momentum-projected wave function is given by

$$|\Phi^I_M\rangle = \sum_k f_k \hat{P}^I_{MK} |\phi_k\rangle \,, \tag{1}$$

where k labels the basis states, and $\hat{P}^I_{MK}$ is the angular momentum projection operator which is explicitly given in Ref. [10]. Acting on intrinsic states, operator $\hat{P}^I_{MK}$ generates the states with a good angular momentum, thus restoring the necessary rotational symmetry violated by the deformed mean field. In this way, the new shell model basis is constructed in which the Hamiltonian is diagonalized; this shell model basis taken in the present paper is as follows:

$$\hat{P}^I_{MK} |\phi_k\rangle \,. \tag{2}$$

Three major shells ($N = 2, 3, 4$) for both the neutron and proton are used and the shell model space includes the zero-, two-, and four-quasiparticle (qp) states:

$$|\phi_k\rangle = \left\{ |0\rangle,\, \alpha^+_{n_i}\alpha^+_{n_j}|0\rangle,\, \alpha^+_{p_i}\alpha^+_{p_j}|0\rangle,\, \alpha^+_{n_i}\alpha^+_{n_j}\alpha^+_{p_i}\alpha^+_{p_j}|0\rangle \right\}, \tag{3}$$

where α^+ is the creation operator for a qp and the index n(p) denotes the neutron (proton) Nilsson quantum numbers which run over the low-lying orbitals. The corresponding qp vacuum is $|0\rangle$. The indices n and p in Eq. (3) are general, for example, a 2-qp state can be of positive (or negative) parity if both quasiparticles i and j are from the same (or two neighboring) major shell(s). Positive and negative parity states span the entire configuration space with the corresponding matrix in a block-diagonal form classified by parity. Since the axial symmetry is kept for the Nilsson states, K is a good quantum number. It can be used to label the basis states in Eq. (3).

The eigenvalue equation of the PSM for a given spin I takes the form

$$\sum_{k'} \{H^I_{kk'} - E^I N^I_{kk'}\} F^I_{k'} = 0 \,, \tag{4}$$

where the Hamiltonian and norm matrix elements are respectively defined by

$$H^I_{kk'} = \langle\phi_k|\,\hat{H}\hat{P}^I_{KK'}\,|\phi_{k'}\rangle\,, \quad N^I_{kk'} = \langle\phi_k|\,\hat{P}^I_{KK'}\,|\phi_{k'}\rangle\,. \tag{5}$$

The expectation values of the Hamitonian with respect to a "rotational band k" H^I_{kk}/N^I_{kk} are called the band energies. When they are plotted as functions of spin I, they form a band diagram [9]. This usually provides us with a useful tool for interpreting band crossings.

The Hamiltonian employed in the PSM calculations contains the separable forces and can be expressed as $\hat{H}=\hat{H}_\nu+\hat{H}_\pi+\hat{H}_{\nu\pi}$ [13], where $\hat{H}_\tau(\tau=\nu,\pi$ and ν denotes neutrons, and π protons) is the like-particle pairing plus quadrupole Hamiltonian, with the inclusion of quadrupole pairing,

$$\begin{aligned}\hat{H}_\tau \;=\; & \hat{H}^0_\tau-\frac{1}{2}\chi_{\tau\tau}\sum_\mu \hat{Q}^{+\mu}_\tau\hat{Q}^\mu_\tau- \\ & G^\tau_M\hat{P}^+_\tau\hat{P}_\tau-G^\tau_Q\sum_\mu\hat{P}^{+\mu}_\tau\hat{P}^\mu_\tau,\end{aligned} \tag{6}$$

and $\hat{H}_{\nu\pi}$ is the n-p quadrupole-quadrupole residual interaction

$$\hat{H}_{\nu\pi}=-\chi_{\nu\pi}\sum_\mu\hat{Q}^{+\mu}_\nu\hat{Q}^\mu_\pi\,. \tag{7}$$

Here $\hat{H}^0_\tau$ is the spherical single-particle Hamiltonian which contains a proper spin–orbit force [14]. The other terms in Eq. (6) are quadrupole–quadrupole, and monopole- and quadrupole-pairing interactions, respectively. The strengths of the quadrupole–quadrupole force $\chi_{\tau\tau}$ $(\tau=\nu,\pi)$ are related self-consistently to the quadrupole deformation ε_2 by

$$\chi_{\tau\tau}=\frac{\frac{2}{3}\varepsilon_2(\hbar\omega_\tau)^2}{\hbar\omega_\nu\left\langle\hat{Q}_0\right\rangle_\nu+\hbar\omega_\pi\left\langle\hat{Q}_0\right\rangle_\pi}\,. \tag{8}$$

Following Ref. [9], the strength $\chi_{\nu\pi}$ is assumed to be

$$\chi_{\nu\pi}=(\chi_{\nu\nu}\chi_{\pi\pi})^{1/2}\,. \tag{9}$$

Similar parametrizations were used in much of the earlier work [15].

The monopole-pairing force constants G_M are

$$G_M=\left[20.12\mp13.13\frac{N-Z}{A}\right]A^{-1}\,, \tag{10}$$

with "−" for neutrons and '+'" for protons, which reproduce the known odd-even mass differences. Finally, the strength parameter G_Q for the quadrupole pairing was simply assumed to be proportional to G_M with a proportionality constant γ, as commonly used in PSM calculations [9]

$$\left(\frac{G_Q}{G_M}\right)_\nu=\left(\frac{G_Q}{G_M}\right)_\pi=\gamma\,. \tag{11}$$

The proportionality constant γ is fixed to be 0.16 in the present calculations (see Table 1).

Additionally, in our calculations, the following four-point formulae are used to calculate the pairing gap parameters $\Delta_{\rm p}$ and $\Delta_{\rm n}$ [16]:

$$\begin{aligned}\Delta_{\rm p} \;=\; & \frac{1}{4}\{B(N,Z-2)-3B(N,Z-1)+ \\ & 3B(N,Z)-B(N,Z+1)\},\end{aligned} \tag{12}$$

$$\begin{aligned}\Delta_{\rm n} \;=\; & \frac{1}{4}\{B(N-2,Z)-3B(N-1,Z)+ \\ & 3B(N,Z)-B(N+1,Z)\}.\end{aligned} \tag{13}$$

The values of the total nuclear binding energy B are taken from Ref. [17]. The results for each nucleus are given in Table 1. The values of the hexadecapole deformation parameter ε_4 taken from the compilation of Möller et al. [18] are also presented in Table 1. The spin-orbit force parameters, κ and μ, appearing in the Nilsson potential are taken from the compilation of Sun et al. [19], which is a modified version of Bengtsson and Ragnarsson [20] and has been fitted to the latest experimental data for proton-rich nuclei with proton or neutron numbers $28\leqslant N\leqslant40$.

Table 1. The relevant parameters used in the PSM.

nuclei	$\Delta_{\rm p}$/MeV	$\Delta_{\rm n}$/MeV	$\gamma=G_Q/G_M$	ε_4
^{80}Zr	1.7935	1.9225	0.16	0.087
^{82}Zr	1.4645	1.5400	0.16	0.000
^{84}Zr	1.5845	1.5325	0.16	0.000

Finally in this section let us briefly introduce the method of calculation of the angular momentum projected potential energy surfaces (AMPPES). The Hamiltonian of the PSM in Eq. (6) does not contain the Coulomb interaction of protons which is indispensable for the potential energy surfaces. To remedy this shortcoming of the PSM and compute the AMPPES we combine the PSM with the RHB theory [21,22]. We first calculate the PES with zero angular momentum based on the RHB theory with the NL3 [23] effective interaction for the relativistic mean-field (RMF) effective Lagrangian and Gogny D1S effective pairing interaction [24,25]. Then we calculate the PES with a given angular momentum in the framework of the PSM. Finally, the energy difference between the PSM calculated PES with a nonzero angular momentum and that with zero spin is added to the RHB calculated PES, and a new PES is formed. Those new PES together with the RHB calculated PES form a group of PES with given angular momenta.

3 Results and discussion

In Section 2, we give most of the parameters used in our calculations. It is still necessary to show that the configuration space is constructed for these nuclei by selecting the qp states close to the Fermi energy in the $N=4$ major shell for both neutrons and protons, and forming multi-qp states from them. The dimension of the qp basis is around 100. We would mention that all calculations in this paper are for positive-parity states.

The mass $A\approx 80$ region is often characterized by shape coexistence. The shape evolution of Zr isotopes is rather involved. The reasons are as follows: (a) For Zr isotopes, many neutrons and protons are distributed in the pfg orbitals, the competition between single-particle motion and collective motion is quite drastic, the level density is so high that the nuclear structure is complicated; (b) There are high-j $g_{9/2}$ intruder orbitals. In Fig. 1, we show the projected PES (the detailed method is described in Section 2) for Zr isotopes ^{80}Zr, ^{82}Zr and ^{84}Zr. These are energies with different angular momenta ($I=0, 2, \cdots$) calculated as functions of deformation ε_2, varying from negative values (corresponding to oblate shapes) to positive values (corresponding to prolate shapes). The multiple shapes are clearly observed for the Zr isotopes. Thereinto, a prolate-spherical-oblate shape coexistence is exhibited in ^{80}Zr and ^{82}Zr, and a spherical-oblate shape coexistence in ^{84}Zr. Usually, a prolate-oblate shape coexists in the other $A\approx 80$ isotopes. The appearance of the exotic shape coexistences in the Zr isotopes is due to the big subshell gap at $Z=40$. The subshell is considered as the spherical subshell [26]. In addition, pronounced superdeformations at $\varepsilon_2\approx 0.55$ appear in ^{82}Zr and ^{84}Zr as is shown in Fig. 1. In 1995, Baktash et al. [27] provided the first evidence for the existence of a new region of high-spin superdeformation ($\beta_2\approx 0.55$) in medium-mass nuclei from Sr to Zr isotopes with particle numbers $N, Z\approx 40$. However, positive-parity superdeformed bands in ^{82}Zr and ^{84}Zr have not yet been reported so far. We look forward to the relevant experimental observation in future.

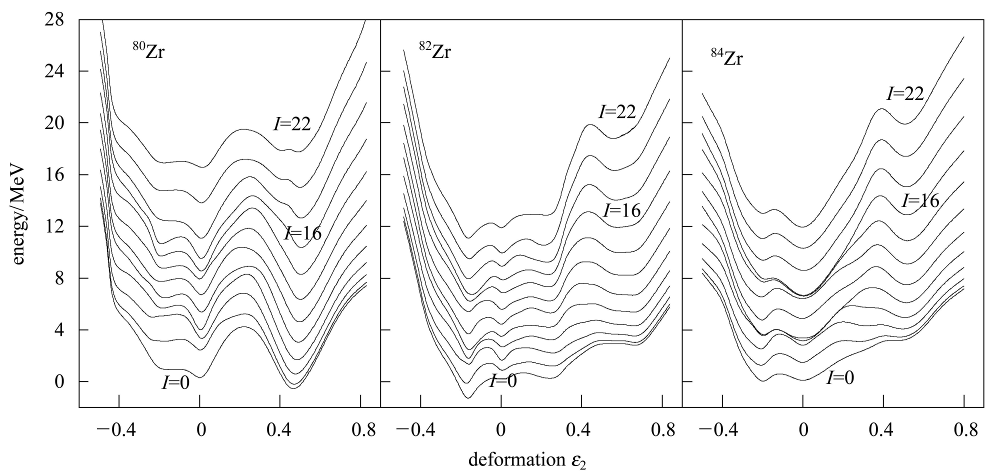

Fig. 1. Projected potential energy surfaces for various spins as functions of deformation variable ε_2 for nuclei ^{80}Zr, ^{82}Zr and ^{84}Zr. The zero energy is set to be the total energy at $\varepsilon_2=0$ and $I=0$.

From the PES curves, we can also determine the shapes of ground states (the lowest minima) for the three nuclei. For ^{80}Zr, the shape of the ground state is strongly prolate (ε_2=0.475), and the potential energy drops sharply. Although the experimental data are rather limited for ^{80}Zr, the rotational band built on the ground state suggests the presence of a large quadrupole deformation [2]. This point of view is consistent with several theoretical results [26,28,29]. The excited state with spin I=0 at the spherical minimum, which may be considered as a shape isomer, is located only 0.65 MeV higher than the ground state. Interestingly, with spin increasing, the spherical minimum becomes lower than the minimum at ε_2=0.475. As a result, a shape phase transition seems to occur around I= 12–16. It would be nice if in future more experimental data would be available to pin down the shape phase transition. Moreover, the shape of the ground state is oblate (ε_2=−0.175) for ^{82}Zr and (ε_2=−0.20) for ^{84}Zr. The structure of ^{84}Zr is similar to that of ^{82}Zr. Why does the structure of ^{80}Zr greatly differ from that of its adjacent nuclei ^{82}Zr and

^{84}Zr?

Let us now examine the shell structure of the three nuclei. One can find the neutrons and protons are mainly distributed in the pf-shell, and all the pf orbitals are filled for ^{80}Zr. The subshell gap at $N=Z=40$ is very large. The large deformation in ^{80}Zr may stem from the valence nucleons being located in the middle of the strongly mixed pf and $g_{9/2}$ shells. However, for $N=Z+2$ nucleus ^{82}Zr and $N=Z+4$ nucleus ^{84}Zr, minority of neutrons are located at $g_{9/2}$ orbitals. These valence neutrons likely drive the collective excitation.

Besides, the n-p interaction is expected to be important for nuclei where protons and neutrons occupy the same major shells because of the large overlaps between proton and neutron single-particle wave functions. Here, we investigate in a purely phenomenological manner the influence of the n-p interaction, through the n-p QQ term [see Eq. (7)] in PSM. It should be noted that the strengths of the proton-proton and neutron-neutron QQ [$\chi_{\pi\pi}$ and $\chi_{\nu\nu}$ in Eq. (6)] are still determined by the self-consistency condition in Eq. (8); we are allowed only to change the n-p strength $\chi_{\nu\pi}$. This method was adopted in Refs. [4,5] and succeeded in interpreting the "delay alignment" in $N=Z$ nuclei. The standard strength of the n-p QQ given by Eq. (9) is based on the assumption of the isoscalar coupling. The implication of our treatment here is that this assumption may not be valid in general, and may be modified by the residual n-p interaction. The details of this method are given in Ref. [5].

In the calculations of the projected PES mentioned above, we have obtained the shapes of ground states of ^{80,82,84}Zr. At a deformed potential, the high-j $g_{9/2}$ orbitals intrude into the pf-shell near the Fermi levels. Therefore, the $g_{9/2}$ orbitals dominate the low-lying structure of these nuclei. In our calculations of the ground state bands, the configuration space is constructed by selecting the qp states close to the Fermi energy in the N=4 (N=4) major shell for neutrons (protons), i.e., K=1/2, 3/2, 5/2, 7/2 orbitals of the $g_{9/2}$ subshell (K=1/2, 3/2, 5/2, 7/2 orbitals of the $g_{9/2}$ subshell) for ^{80}Zr and all orbitals of the $g_{9/2}$ subshell (K=1/2, 3/2, 5/2, 7/2 orbitals of the $g_{9/2}$ subshell) for both ^{82}Zr and ^{84}Zr respectively, and forming multi-qp states from them.

The calculations of ground state bands for the three nuclei ^{80}Zr, ^{82}Zr and ^{84}Zr are presented in Fig. 2. For each of them, we change the strength $\chi_{\nu\pi}$ by multiplying a factor a=0.6, 0.8, 1.0, 1.3, 1.5. A rather pronounced effect can be seen for ^{80}Zr as is shown in Fig. 2. With increasing the n-p strength, the energies of the ground state bands decrease gradually. When using a=1.3, the results can reproduce the experimental data (up to spin I^{π}=10^{+} so far) well. This n-p strength is consistent with that in Refs. [4,5] which interpreted the delayed rotational alignment in the $N=Z$ nuclei. It gives a signature that a stronger n-p interaction exists in $N=Z$ nuclei ^{80}Zr. A stronger n-p strength such as a=1.5 will result in a disagreement. On the other hand, the calculations with a smaller n-p strength such as a=0.8 give higher values than the experimental data.

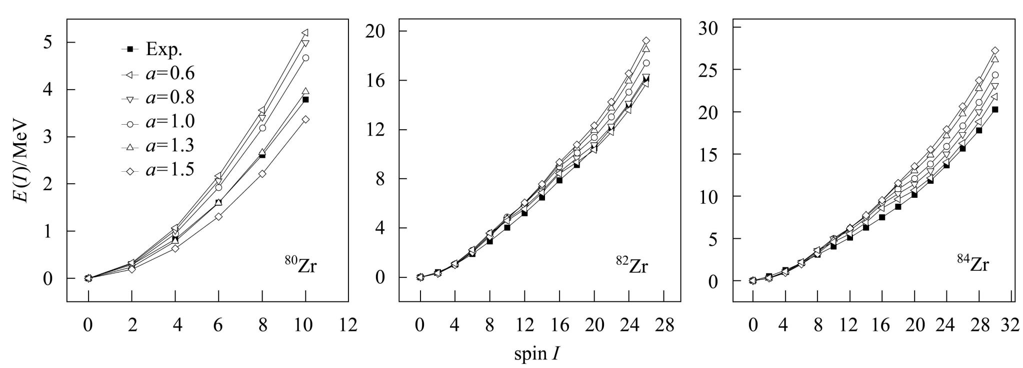

Fig. 2. PSM calculations with various n-p interaction strengths in comparison with the experimental data for the ground state bands in ^{80}Zr, ^{82}Zr and ^{84}Zr. The experimental data are taken from Ref. [2] for ^{80}Zr, Ref. [30] for ^{82}Zr and Ref. [31] for ^{84}Zr.

For the other two adjacent nuclei ^{82}Zr and ^{84}Zr, it can be seen that the effect of the n-p interaction is not so pronounced for low spins ($I \leqslant 16$). But at higher spins, the energies of these states increase gradually with increasing n-p strength. This trend is reversed compared with that in ^{80}Zr. Moreover, we find that our calculations are in good agreement with the experimental data when using a=0.8 for ^{82}Zr, and when using a=0.6 for ^{84}Zr (see Fig. 2). This suggests that the n-p interaction strength decreases as the number of neutrons increases for the three Zr isotopes. It is well known that the PSM approach with the standard n-p strength (a=1.0) is an excellent tool to calculate the nuclear collective rotations [9]. In general, however, the PSM calculated values at high spins are a little bit higher than the experimental data. This is attributed to the limitation of the PSM. For example, the shell model space could include only up to four-quasiparticle states in the present PSM code. Hence, we are not sure that a decreasing n-p strength exists in ^{82}Zr and ^{84}Zr. Maybe the standard n-p strength (a=1.0) has already given the results in good agreement with the experiments for ^{82}Zr and ^{84}Zr. However, the n-p interaction in ^{80}Zr is obviously much stronger than that in the other two nuclei ^{82}Zr and ^{84}Zr though they are its adjacent nuclei. This means that the effect of the n-p interaction in the $N = Z$ nuclei is quite different from that in the $N \neq Z$ nuclei. This is probably due to the imbalance of the numbers of neutrons and protons. The stronger n-p interaction in the $N = Z$ nucleus is perhaps responsible for the sudden change of the rotational alignment with an increase or a decrease of its nucleon number by only one or two.

All our calculations and discussions predict that $N = Z$ nuclei have their own specific features. The residual n-p interaction which is supposed to be important for the $N = Z$ systems should be of pairing type. It has been found from several mean-field studies (see, for example, Ref. [32]) that the n-p paring is nonzero for $N = Z$ nuclei and vanishes for $N \neq Z$ nuclei. However, the n-p pairing contains pairs of higher angular momenta [33] apart from J=1 pairs. These higher angular momenta pairs will have a significant particle-hole contribution and may modify, for example, the QQ interaction used in the PSM Hamiltonian. Therefore, increasing the strength of the QQ term in the n-p interaction, as has been done in the present work, has a physics origin. It is interesting to see that the n-p pairing term tends to renormalize the QQ interaction for the $N = Z$ nucleus only in the PSM, but for the $N \neq Z$ nuclei a change of the strength would not affect the results so much.

4 Conclusions

In the present paper, we have investigated the nuclear structure near the $N = Z$ line. Based on the PSM together with the RHB theory, we calculated the projected PES for various spins for three Zr isotopes ^{80,82,84}Zr. From the projected PES, we have obtained the following results: (1) Shape coexistence exhibits in all three nuclei; (2) Pronounced super-deformations ($\varepsilon_2 \approx 0.55$) occur in ^{82}Zr and ^{84}Zr; (3) The ground state is of strongly prolate shape for the $N = Z$ nucleus ^{80}Zr ($\varepsilon_2 = -0.475$), and of oblate shape both for ^{82}Zr ($\varepsilon_2 = -0.175$) and for ^{84}Zr ($\varepsilon_2 = -0.20$) respectively. In addition, by means of calculations of the ground state band for these nuclei using the PSM, this shows that the residual n-p interaction plays a more important role in the structure of the $N = Z$ nucleus ^{80}Zr compared with its nearest neighbors ^{82,84}Zr.

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