

Abnormal Bifurcation of the Double Binding Energy Differences and Proton-Neutron Pairing: Nuclei Close to $N=Z$ Line from Ni to Rb

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The recently observed abnormal bifurcation of the double binding energy differences δV_{pn} between the odd-odd and even-even nuclei along the $N = Z$ line from Ni to Rb has challenged the nuclear theories. To solve this problem, a shell-model-like approach based on the relativistic density functional theory is established, by treating simultaneously the neutron-neutron, proton-neutron, and proton-proton pairing correlations both microscopically and self-consistently. Without any *ad hoc* parameters, the calculated results well reproduce the observations, and the mechanism for this abnormal bifurcation is found to be due to the enhanced proton-neutron pairing correlations in the odd-odd $N = Z$ nuclei, compared with the even-even ones. The present results provide an excellent interpretation for the abnormal δV_{pn} bifurcation, and provide a clear signal for the existence of the proton-neutron pairing correlations for nuclei close to the $N = Z$ line.

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The double binding energy difference δV_{pn} , is an important mass filter for atomic nuclei, and has been frequently used to isolate the residual proton-neutron (pn) interaction [1,2]. It is closely related to many nuclear structure phenomena, such as the onset of collectivity and deformation [3–6], the evolution of the underlying shell structure [7], and the phase transition behavior in nuclei [4,8]. The study of δV_{pn} , particularly along the line of the nuclei with equal numbers of protons and neutrons, is of great importance to deepen our understanding of the nuclear force [9]. For example, the considerable enhancement of δV_{pn} for $N = Z$ nuclei in the light sd shell has been regarded as the fingerprint for the Wigner’s SU(4) symmetry of the nuclear force [10]. For heavier nuclei in the sd shell and even lower fp shell, the decrease of δV_{pn} with mass number is related to the breaking of the Wigner’s SU(4) symmetry due to the increasing spin-orbit and Coulomb interactions.

For the upper fp -shell nuclei, however, the δV_{pn} shows quite puzzling behavior. On one hand, restrengthening δV_{pn} values have been observed [11,12] for the odd-odd nuclei, and this phenomenon might be attributed to the restoration of the pseudo-SU(4) symmetry [13], the enhanced overlaps of the proton and neutron wave functions [14–16] or the nuclear deformation [6,17]. On the other hand, a recent experiment has reported an abnormal bifurcation, namely, opposite evolving trends of δV_{pn} with mass number for the even-even and odd-odd $N = Z$ nuclei from Ni to Rb [18], which cannot be understood by the aforementioned physical mechanisms and, thus, brought severe challenges to the theoretical models, including the macroscopic-microscopic

models [19–23], the shell model [24], and the density functional theories (DFTs) [25–27]. Note that the macroscopic-microscopic models and DFTs are quite successful for a global description of nuclear masses over the whole nuclear chart. Their failure in describing the observed δV_{pn} bifurcation indicates that important physics may be missing in the current nuclear models.

The valence-space in-medium similarity renormalization group calculations imply that the three-nucleon force has a significant impact on the behavior of δV_{pn} , but the obtained amplitudes of the δV_{pn} bifurcation between the even-even and odd-odd $N = Z$ nuclei are dramatically overestimated [18]. The inclusion of a phenomenological Wigner term in the macroscopic-microscopic models [19–23] and DFT [27] also results in a δV_{pn} bifurcation between the even-even and odd-odd $N = Z$ nuclei, but the δV_{pn} for the odd-odd nuclei are systematically underestimated [18].

For $N = Z$ nuclei, it is very important to take into account the pn pairing correlations. In particular, for odd-odd $N = Z$ nuclei, the last valence neutron and proton could be paired due to the pn pairing correlations, which are responsible for the phenomenological Wigner terms [28–31]. To solve the puzzle of the δV_{pn} bifurcation, a microscopic model which could treat the neutron-neutron (nn), proton-proton (pp), and pn pairing correlations simultaneously and self-consistently is necessary. The blocking effects for odd-odd nuclei should be treated carefully.

The nuclear DFT starts from a universal density functional and has achieved great successes in describing many nuclear phenomena [32–37]. It is a promising framework to consider the pn pairing correlations in a microscopic way.

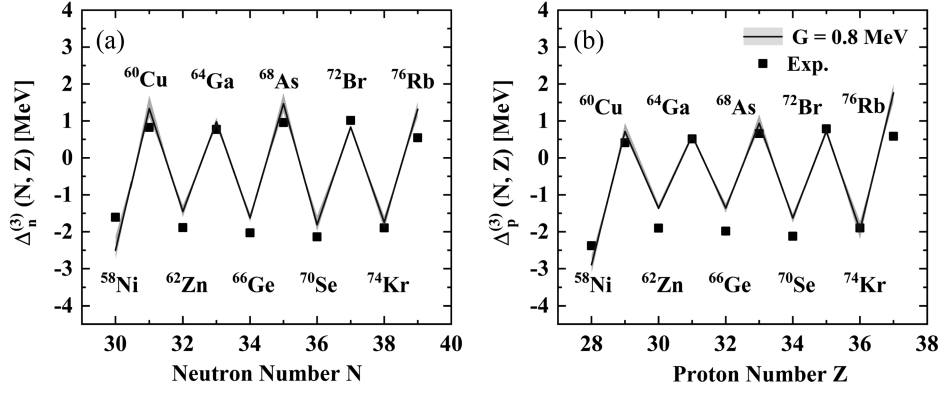


FIG. 1. Odd-even mass differences $\Delta_n^{(3)}$ (a) and $\Delta_p^{(3)}$ (b) for the $N = Z + 2$ nuclei from Ni to Rb calculated by RDFT-SLAP (lines) in comparison with the data (symbols). The gray bands correspond to the odd-even mass differences for the pairing strength G varying by 10%.

In the conventional Bardeen-Cooper-Schrieffer and Bogoliubov methods, the particle number conservation is violated and the Pauli blocking effects in odd-nucleon systems cannot be treated exactly [38]. The shell-model-like approach (SLAP), also known as particle number conserving method, treats the pairing correlations and the blocking effects exactly by diagonalizing the many-body Hamiltonian in a properly truncated many-particle configuration (MPC) space with good particle number [39,40]. It has been implemented in the relativistic [41–46] and nonrelativistic [47,48] DFTs to treat the nn and pp pairing correlations and widely used to investigate both the nuclear ground-state and excited-state properties. Nevertheless, a self-consistent treatment of the pn pairing correlations is missing.

In this Letter, based on the relativistic DFT (RDFT), a SLAP is developed, which allows a microscopic and self-consistent treatment of the nn , pp , and pn pairing correlations simultaneously. The developed approach will be applied to investigate the abnormal δV_{pn} bifurcation for the $N = Z$ nuclei from Ni to Rb.

In the SLAP based on RDFT (RDFT-SLAP), the many-body Hamiltonian reads

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{pair}}, \quad (1)$$

where \hat{H}_0 is the one-body part, and \hat{H}_{pair} is the pairing part. The one-body part reads

$$\hat{H}_0 = \sum_{k>0} [e_k^\pi (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) + e_k^\nu (b_k^\dagger b_k + b_{\bar{k}}^\dagger b_{\bar{k}})], \quad (2)$$

where \bar{k} represents the time conjugate of the state k , and $e_k^{\pi(\nu)}$ are the single-proton (neutron) energies obtained from the Dirac equation,

$$[-i\alpha \cdot \nabla + \beta(m + S) + V]\psi_k = e_k \psi_k. \quad (3)$$

Here, the scalar field S and vector field V are connected in a self-consistent way to the scalar and vector densities, for details see Ref. [41]. The pairing part reads

$$\hat{H}_{\text{pair}} = \sum_{T_z=0,\pm 1} \hat{H}_{\text{pair}}^{T_z}, \quad \hat{H}_{\text{pair}}^{T_z} = -G \sum_{\substack{k \neq k' \\ k, k' > 0}} P_{k, T_z}^\dagger P_{k', T_z}, \quad (4)$$

where G is the effective pairing strength, and $k \neq k'$ means that the self-scattering for the nucleon pairs is forbidden [41]. The nn and pp pair creation operators are $P_{k,1}^\dagger = b_k^\dagger b_{\bar{k}}^\dagger$ and $P_{k,-1}^\dagger = a_k^\dagger a_{\bar{k}}^\dagger$ for $T_z = \pm 1$, and the pn pair creation operator is $P_{k,0}^\dagger = (1/\sqrt{2})(b_k^\dagger a_{\bar{k}}^\dagger + a_k^\dagger b_{\bar{k}}^\dagger)$ for $T_z = 0$.

The nuclear wave functions are expressed as

$$|\Psi\rangle = \sum_{i, \{s_k\}} C_i^{\{s_k\}} |\text{MPC}_i^{\{s_k\}}\rangle. \quad (5)$$

The many-particle configurations $|\text{MPC}_i^{\{s_k\}}\rangle$ with exact proton number Z and neutron number N are expressed as $|l_1 l_2 \cdots l_N m_1 m_2 \cdots m_Z\rangle = b_{l_1}^\dagger b_{l_2}^\dagger \cdots b_{l_N}^\dagger a_{m_1}^\dagger a_{m_2}^\dagger \cdots a_{m_Z}^\dagger |0\rangle$, and the corresponding configuration energy is denoted as E_i . Here, s_k represents the eigenvalue of the seniority operator \hat{s}_k for the state k [49], and it is a good quantum number. The expansion coefficients $C_i^{\{s_k\}}$ and, thus, the wave functions are determined by diagonalizing the Hamiltonian \hat{H} in the MPC space.

Note that the obtained wave function $|\Psi\rangle$ is used to determine the occupation probabilities for the single-particle states, and thus the nucleon densities should be updated, which in turn determines the scalar and vector fields S and V in the Dirac equation (3). Therefore, the full framework should be solved iteratively to achieve the self-consistency [41,44,45]. Once a self-consistent solution is obtained, one can calculate the pairing energy,

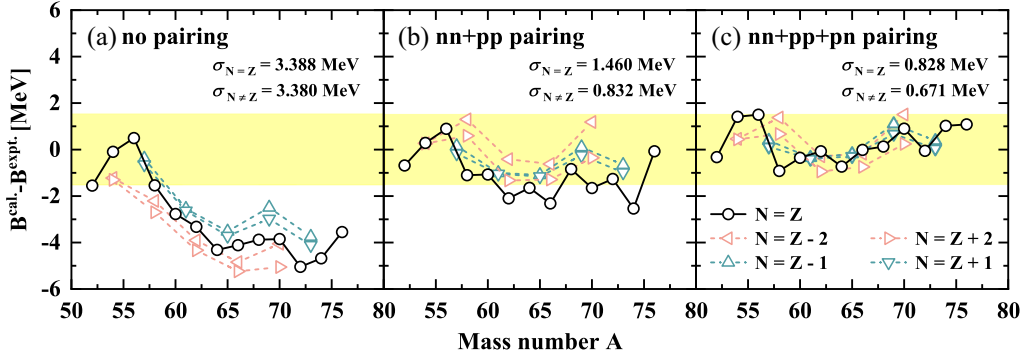


FIG. 2. Differences between the calculated binding energies and the data for the $N = Z, Z \pm 1, Z \pm 2$ nuclei around Ni and Rb region without pairing (a), with the n - n and pp pairing (b), and with the nn , pp , and pn pairing (c). The root-mean-square deviation for the $N = Z$ ($N \neq Z$) nuclei $\sigma_{N=Z}$ ($\sigma_{N \neq Z}$) is also given.

$$E_{\text{pair}} = \langle \Psi | \hat{H}_{\text{pair}} | \Psi \rangle = \sum_{ij} C_i^* C_j \langle \text{MPC}_i | \hat{H}_{\text{pair}} | \text{MPC}_j \rangle, \quad (6)$$

which is added to the total energy of RDFT.

In this work, the relativistic density functional PC-PK1 [50] is adopted. The Dirac equation (3) is solved in the three-dimensional harmonic oscillator basis in Cartesian coordinates [51] with ten major shells, and the quadrupole deformation including triaxiality is considered self-consistently.

The dimension of the MPC space and the corresponding pairing strength G are determined by the odd-even mass differences of the $N = Z + 2$ nuclei from Ni to Rb. In Fig. 1, the calculated odd-even mass differences $\Delta_n^{(3)}(N, Z) = [B(N-1, Z) + B(N+1, Z)]/2 - B(N, Z)$ and $\Delta_p^{(3)}(N, Z) = [B(N, Z-1) + B(N, Z+1)]/2 - B(N, Z)$ [52] are shown, in comparison with the experimental ones extracted from AME'20 [53,54]. The experimental odd-even mass differences are well reproduced by the calculation with the pairing strength $G = 0.8$ MeV. The corresponding MPC space is truncated by $E_{\text{cut}} = 16$ MeV, which means only the MPCs with the energies $E_i \leq 16$ MeV are included in the model space. In addition, a variation of the pairing strength by 10% does not change the odd-even mass differences $\Delta_n^{(3)}$ and $\Delta_p^{(3)}$ significantly.

With the pairing strength G thus determined, the binding energies for the $N = Z, Z \pm 1, Z \pm 2$ nuclei around Ni and Rb region are calculated. The differences between the calculated binding energies and the data [53,54] are shown in Fig. 2. As shown in Fig. 2(a), without the pairing correlations, the deviations between the calculated binding energies and the data are large. The root-mean-square (rms) deviations are 3.388 MeV for $N = Z$ nuclei and 3.380 MeV for $N \neq Z$ ones. After the inclusion of the nn and pp pairing, as shown in Fig. 2(b), the descriptions of the binding energies are improved. The rms deviation for $N = Z$ nuclei changes to 1.460 MeV, and for $N \neq Z$ nuclei

changes to 0.832 MeV. After including the pn pairing, as shown in Fig. 2(c), the agreements become better. The rms deviation is 0.828 MeV for $N = Z$ nuclei and 0.671 MeV for $N \neq Z$ nuclei [55]. These results illustrate the importance of the pairing correlations for nuclei near the $N = Z$ line, in particular the pn pairing correlations.

From the binding energies, the δV_{pn} can be extracted as [10]

$$\delta V_{pn}^{\text{ee}}(N, Z) = \frac{1}{4} [B(N, Z) - B(N-2, Z) - B(N, Z-2) + B(N-2, Z-2)], \quad (7)$$

for even-even nuclei with $N = Z$, and

$$\delta V_{pn}^{\text{oo}}(N, Z) = [B(N, Z) - B(N-1, Z) - B(N, Z-1) + B(N-1, Z-1)], \quad (8)$$

for odd-odd nuclei with $N = Z$. The extracted theoretical results and data [18] are shown in Fig. 3. The experimental $\delta V_{pn}^{\text{ee}}$ (red circles) decrease smoothly with the mass number, while the $\delta V_{pn}^{\text{oo}}$ (blue squares) exhibit a distinct tendency; this is the challenging puzzle of the abnormal δV_{pn} bifurcation observed in Ref. [18]. When the nn , pp , and pn pairing correlations are taken into account simultaneously (solid lines), the calculated results well reproduce the evolution of δV_{pn} for both the odd-odd and even-even nuclei. The agreement remains even by changing the pairing strength by 10%. In contrast, if the pn pairing correlations are switched off (dashed lines), the calculated results cannot reproduce the bifurcation. As shown clearly in Fig. 3, the successful reproducing for the abnormal δV_{pn} bifurcation is due to the enhancement of the δV_{pn} for the odd-odd $N = Z$ nuclei by the pn pairing correlations.

To further understand why the pn pairing correlations have more significant influence on the δV_{pn} for the odd-odd nuclei as compared to the even-even ones, in

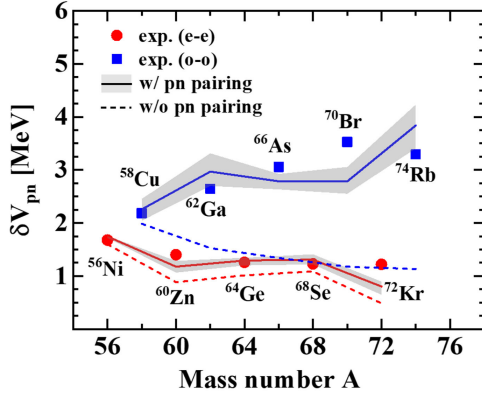


FIG. 3. Calculated δV_{pn} for the even-even (red lines) and odd-odd (blue lines) $N = Z$ nuclei from Ni to Rb with (solid lines) and without (dashed lines) the pn pairing, in comparison with the data (symbols) [18]. The gray bands correspond to the results with the pairing strength G varying by 10%.

Fig. 4(a), the calculated pn pairing energies, $E_{\text{pair}}^{pn} = \langle \Psi | \hat{H}_{\text{pair}}^{T_z=0} | \Psi \rangle = \sum_{ij} C_i^* C_j \langle \text{MPC}_i | \hat{H}_{\text{pair}}^{T_z=0} | \text{MPC}_j \rangle$, are shown as functions of the sums of the configuration energies for $N = Z$ odd-odd nucleus ^{66}As and even-even nucleus ^{64}Ge . For ^{66}As , the nonvanishing value of E_{pair}^{pn} starts at about 3.5 MeV, while for ^{64}Ge , about 6.9 MeV. This can be understood from the lowest MPC and the lowest excitation contributing to the pn pairing energy for ^{66}As and ^{64}Ge as shown in Figs. 4(b) and 4(c). With the increase of $E_i + E_j$, the pn pairing energy for ^{66}As is significantly larger than that for ^{64}Ge . Changing the pairing strength G by 10% will influence the pn pairing energy by around 1 MeV for ^{66}As ,

and by around 0.4 MeV for ^{64}Ge . These results in Fig. 4 suggest that the pn pairing correlations have more influence on the odd-odd nuclei than on the even-even nuclei, and this explains why the pn pairing correlations would significantly enhance the δV_{pn} for the odd-odd $N = Z$ nuclei in Fig. 3, and thus result in the abnormal δV_{pn} bifurcation.

In summary, a shell-model-like approach is developed based on the relativistic density functional theory, which allows a microscopic and self-consistent treatment of the neutron-neutron, proton-proton, and proton-neutron pairing correlations simultaneously. The challenging puzzle of the abnormal δV_{pn} bifurcation between the odd-odd and even-even nuclei along the $N = Z$ line from Ni to Rb is found to be originated from the proton-neutron pairing correlations. The proton-neutron pairing correlations would significantly enhance the δV_{pn} for odd-odd $N = Z$ nuclei, and thus result in the δV_{pn} bifurcation. The proton-neutron pairing correlations improve the description of the masses not only for $N = Z$ nuclei, but also for these nuclei near the $N = Z$ line. These conclusions remain true even if the pairing strength is changed by 10%. The present results provide an excellent interpretation to the challenging puzzle of the abnormal δV_{pn} bifurcation, and provide a clear signal for the existence of the proton-neutron pairing correlations for $N = Z$ nuclei.

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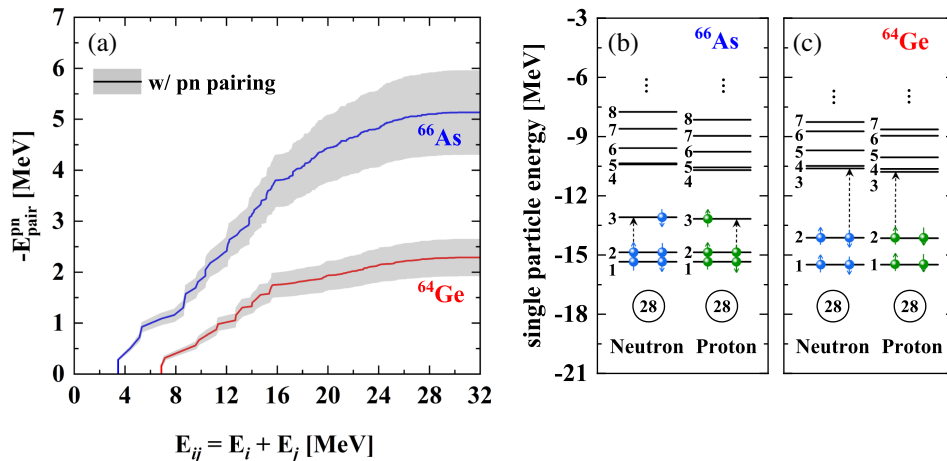


FIG. 4. (a) Calculated pn pairing energies E_{pair}^{pn} as functions of the sums of the configuration energies for the i th and j th MPC, $E_i + E_j$, for ^{66}As and ^{64}Ge . The gray bands correspond to the results for the pairing strength G varying by 10%. (b) Single-particle energies for the odd-odd nucleus ^{66}As . The single-proton levels are renormalized to the first single-neutron level above the $N = Z = 28$ shell. The lowest-energy MPC and the lowest excitation with nonvanishing contribution to the pn pairing energy E_{pair}^{pn} are schematically shown. (c) Same as (b), but for the even-even nucleus ^{64}Ge .

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