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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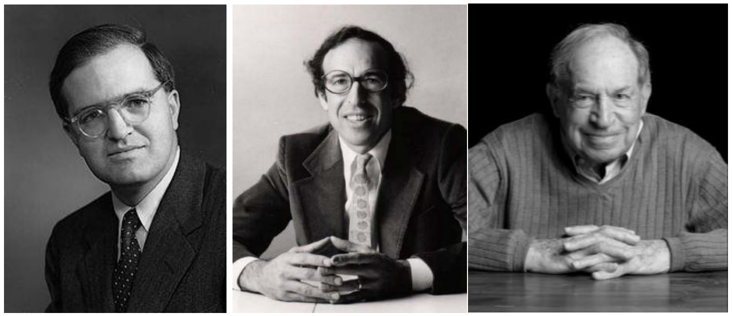
WYP, Y. K. Wang, F. F. Xu, P. W. Zhao, and J. Meng, PRL 132 (2024) 232501

Outline

- Introduction
- Theoretical Framework
- Numerical Details
- Results and Discussions
- Summary and Outlook

Pairing correlations

Proposal

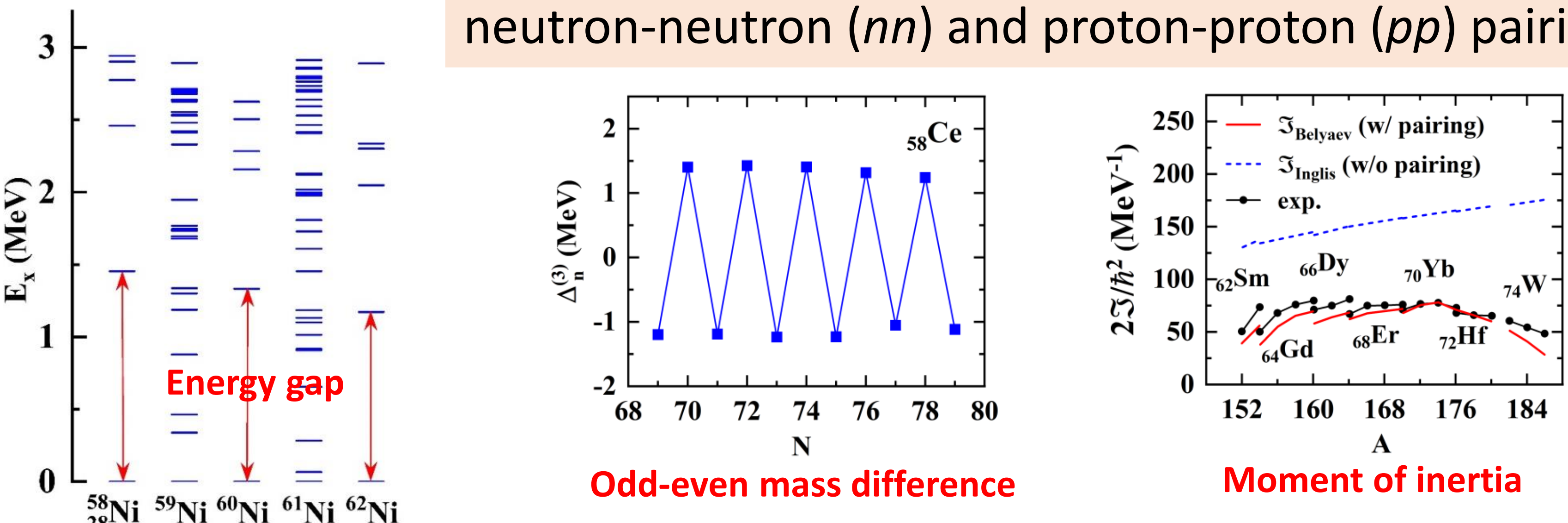


"There is a possible analogy between the excitation spectra of nuclei and those of the superconducting metallic state."

Bohr, Mottelson, Pines, PR 110 (1958) 936

Experimental evidence

neutron-neutron (*nn*) and proton-proton (*pp*) pairing



Odd-even mass difference

Moment of inertia

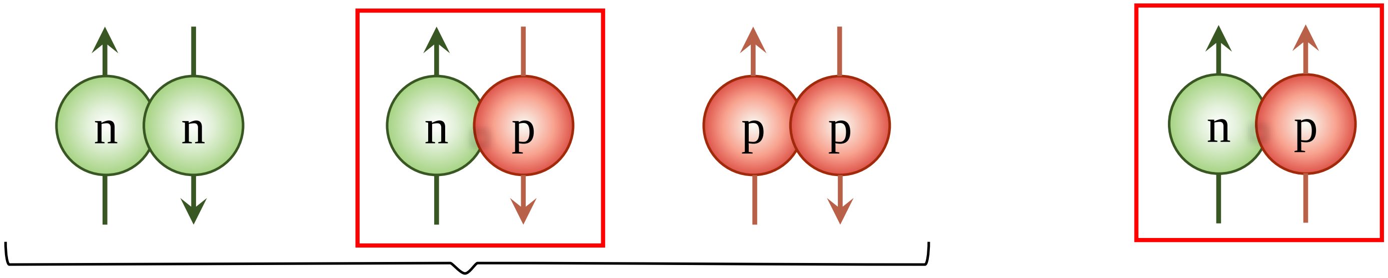
Data from National Nuclear Data Center

Nilsson & Ragnarsson, Shapes and Shells in Nuclear Structure (1995)

Proton-neutron pairing correlations

- In atomic nuclei, the proton-neutron (*pn*) pairing correlations may also exist.

Novel pairing phenomenon not found elsewhere in nature



$T = 1; \quad S = 0; \quad L = 0$

Isovector Pairing

$T = 0; \quad S = 1; \quad L = 0$

Isoscalar Pairing

- Issues of special interest:
  - **Existence** of *pn* pairing condensates;
  - **Coexistence** of *nn*, *pp* and *pn* pairing condensates;
  - **Different roles** played by isovector and isoscalar pairing correlations.

Frauendorf & Macchiavelli, PPNP 78 (2014) 24

Theoretical studies of *pn* pairing correlations

- Theoretical approaches for the study of *pn* pairing correlations

Exactly Solvable Model

Dukelsky et al., PRL 96 (2006) 072503; Lerma et al., PRL 99 (2007) 032501
Pan, Draayer, PRC 66 (2002) 044314; Romero, Dobaczewski, Pastore, APPB 49 (2018) 347

Shell Model

- Cranked Shell Model Monte Carlo Approach — Dean et al., PLB 399 (1997) 1
- Lanczos Method — Poves & Martinez-Pinedo, PLB 430 (1998) 203
- Projected Shell Model — Sun, EPJA 20 (2004) 133

Phenomenological Mean Field Method

- BCS (Woods-Saxon pot.) + Lipkin-Nogami — Satuła et al., PLB 393 (1997) 1
- Hartree-Bogoliubov (Nilsson pot.) — Bentley et al., PRC 89 (2014) 034302
- Hartree-Fock-Bogoliubov + Excited Vampir Approach — A. Petrovici et al., NPA 647 (1999) 197

Density Funtional Theory (DFT)

- Cranked Skyrme Hartree-Fock-Bogoliubov — Terasaki et al., PLB 437 (1998) 1
- Skyrme Hartree-Fock + Quartet Condensation Model — Negrea, Sandulescu, Gambacurta, PRC 105 (2022) 034325
- Cranked Relativistic Hartree-Bogoliubov + Lipkin-Nogami — Afanasjev & Frauendorf, PRC 71 (2005) 064318

...

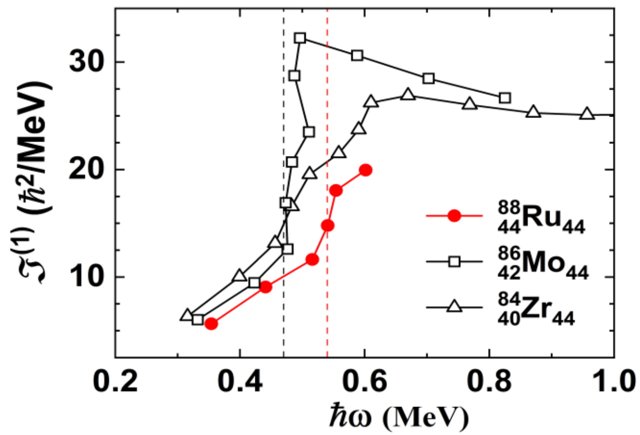
Experimental signals of *pn* pairing correlations

$N = Z$ Nuclei

ideal place to find *pn* pairing signals

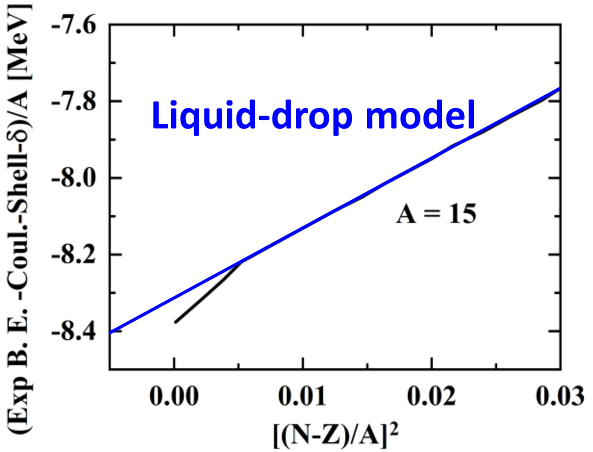
"with enhanced correlations between neutrons and protons that occupy orbitals with the same quantum numbers"

- **Delayed alignment in $N = Z$ nuclei**



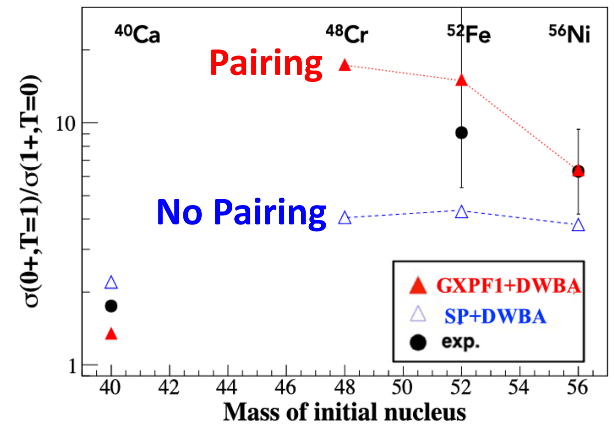
Cederwall et al., Phys. Rev. Lett 124 (2020) 062501

- **Additional binding of $N = Z$ nuclei**



Myers, Swiatecki, Nucl. Phys. 81 (1966) 1

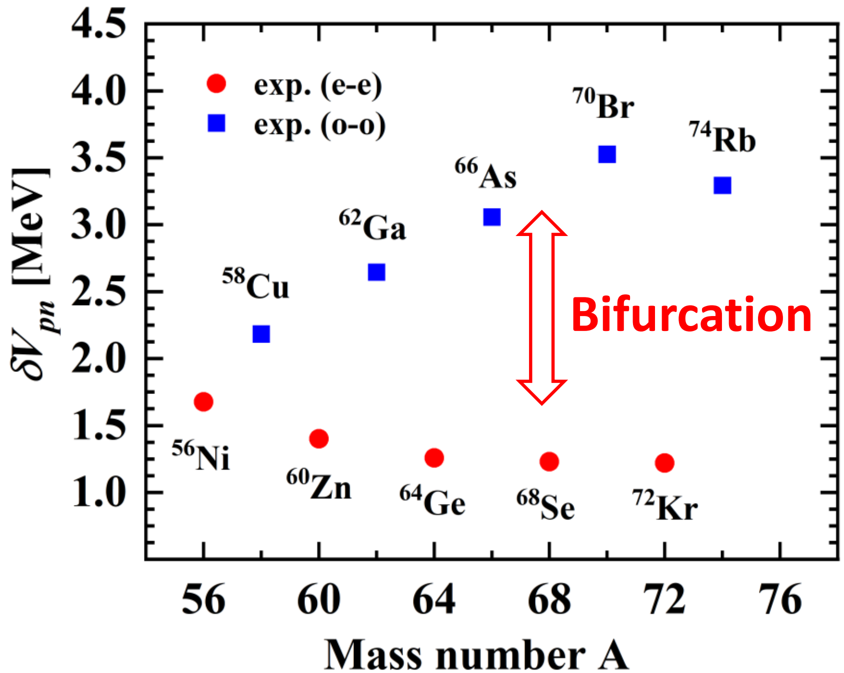
- ***pn* pair transfer cross-section**



Le Crom et al., Phys. Lett. B 829 (2022) 137057

Abnormal bifurcation of δV_{pn} for $N = Z$ nuclei

- State-of-the-art mass measurement reveals an abnormal δV_{pn} bifurcation.



Wang et al., PRL 130 (2023) 192501

Double binding energy difference δV_{pn}

an important mass filter closely related to …

- **Collectivity and deformation**
  Talmi, Rev. Mod. Phys. 34 (1962) 704
  Casten, Phys. Rev. Lett. 54 (1985) 1991
  Cakirli, Casten, Phys. Rev. Lett. 96 (2006) 132501
- **Underlying shell structure**
  Heyde et al., Phys. Lett. B 155 (1985) 303
- **Phase transition behavior**
  Federman, Pittel, Phys. Lett. B 69 (1977) 385
  Federman, Pittel, Phys. Lett. B 77 (1978) 29

$$\delta V_{pn}^{\text{o-o}}(N,Z) = \frac{\partial^2 B}{\partial N \partial Z} = B(N,Z) - B(N-1,Z) - B(N,Z-1) + B(N-1,Z-1)$$

$$\delta V_{pn}^{\text{e-e}}(N,Z) = \frac{\partial^2 B}{\partial N \partial Z} = \frac{1}{4}\left[B(N,Z) - B(N-2,Z) - B(N,Z-2) + B(N-2,Z-2)\right]$$

Van Isacker et al., PRL 74 (1995) 4607

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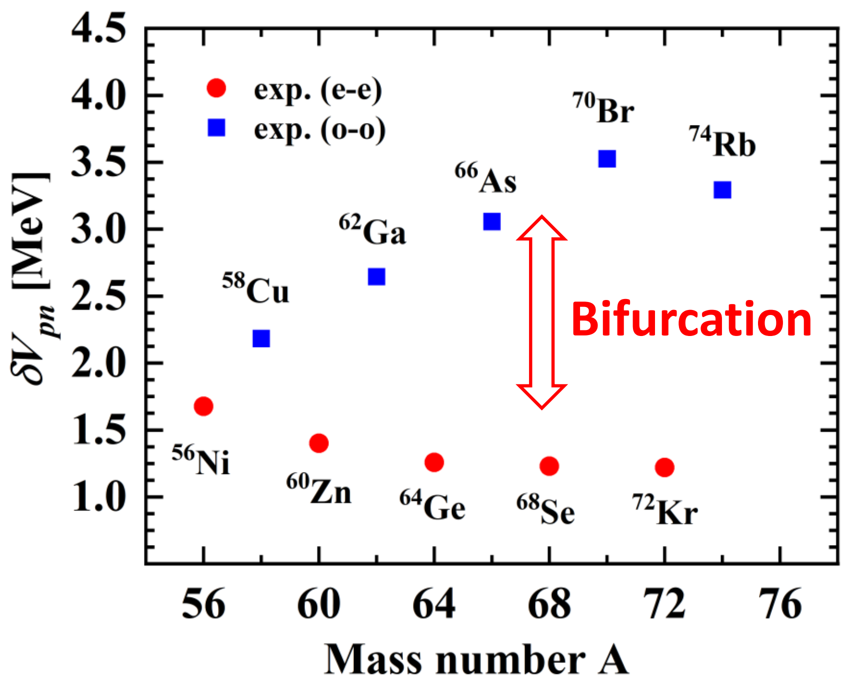
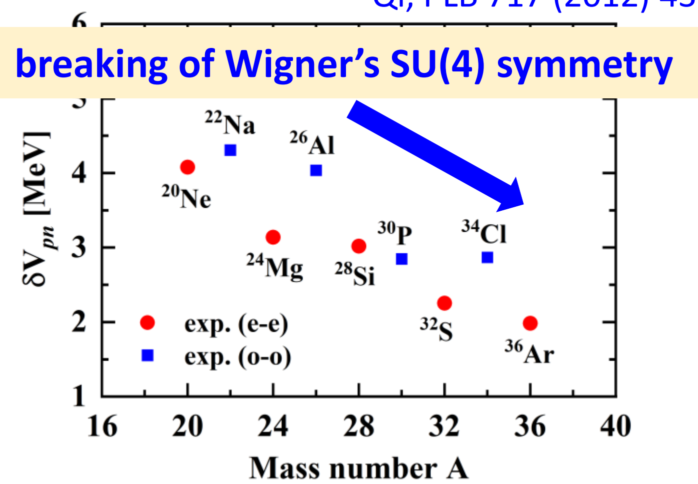


Wang et al., PRL 130 (2023) 192501

Study of δV_{pn} along $N = Z$ line deepens our understanding of nuclear force.

Warner et al., Nat. Phys. 2 (2006) 311
Qi, PLB 717 (2012) 436



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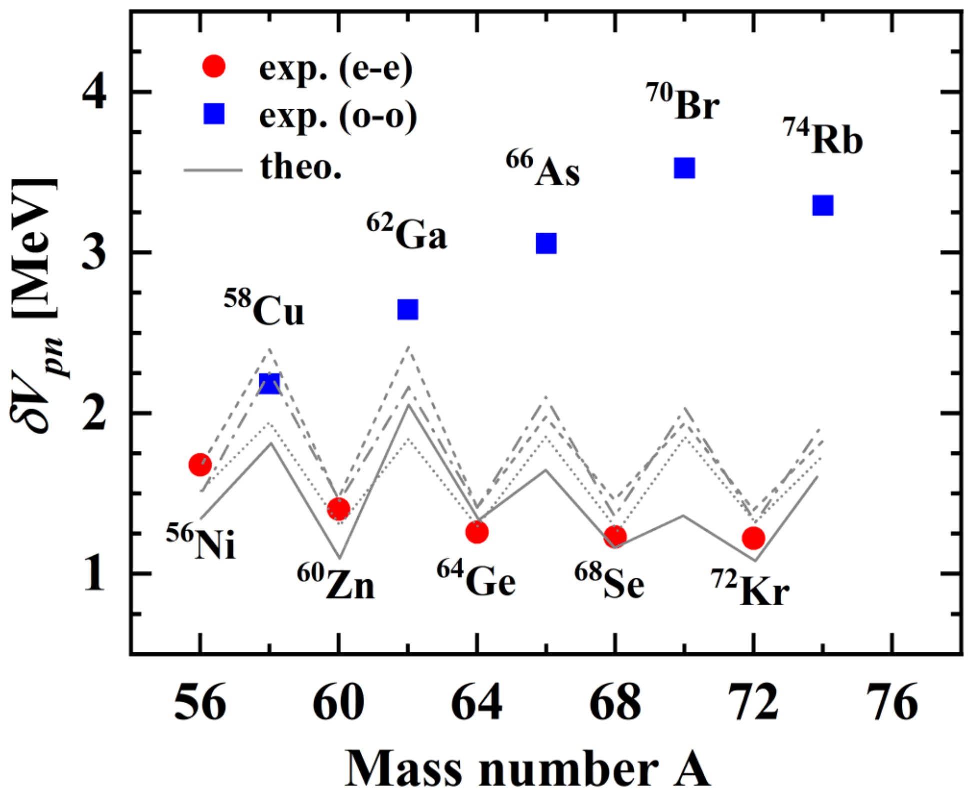
Van Isacker et al., PRL 74 (1995) 4607

Bring challenges to the nuclear theories

- Frequently used mass models (macroscopic-microscopic models, shell model, and **DFTs**) fail to describe the δV_{pn} bifurcation.



Wang et al., PRL 130 (2023) 192501

DZ28 Duflo, Zuker, PRC 52 (1995) R23(R)

WS4 Wang et al., PLB 734 (2014) 215

KTUY05 Kawano et al., JNST 43 (2006) 1

FRDM12 Möller et al., ADNDT 109 (2016) 1

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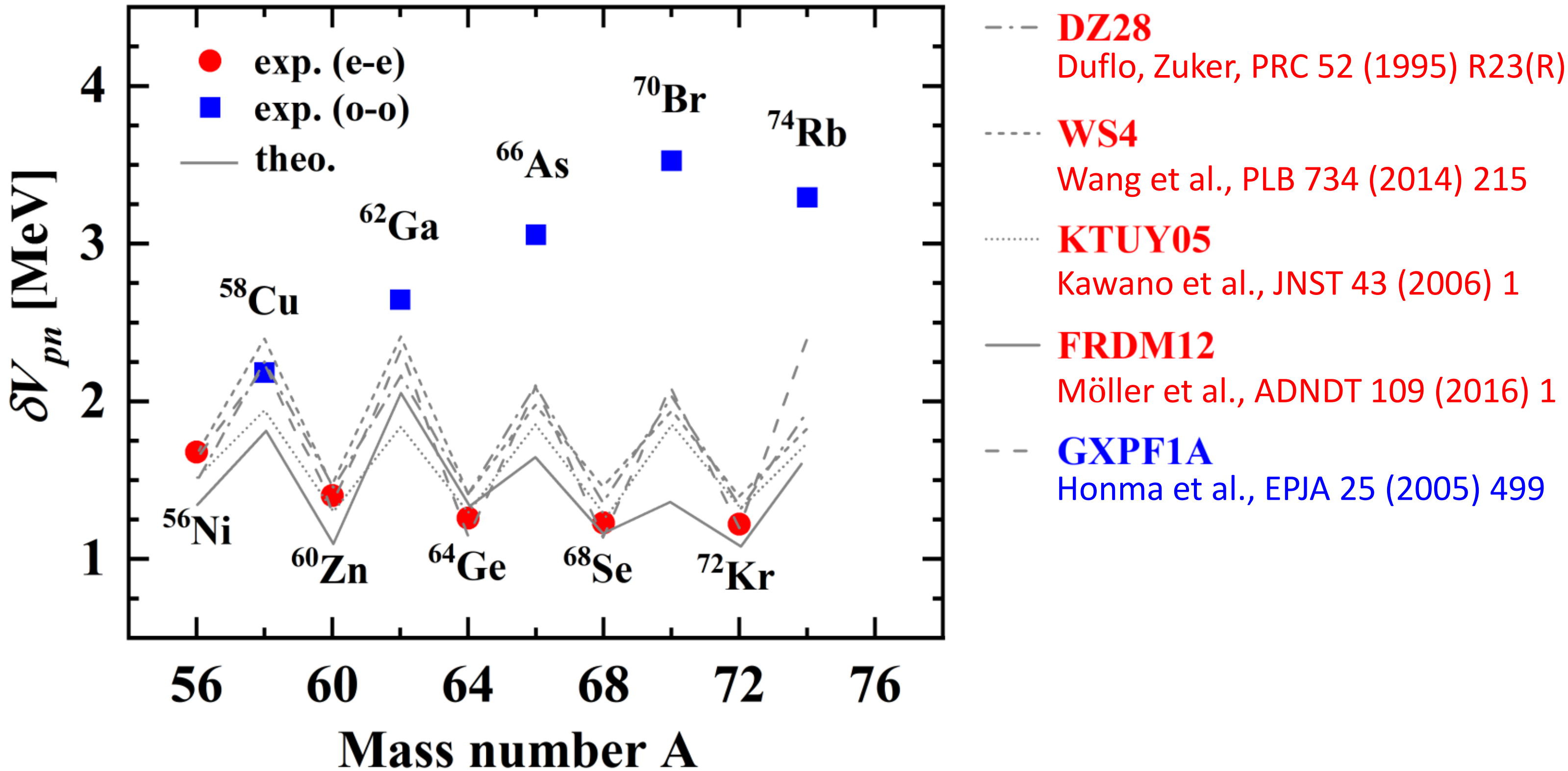

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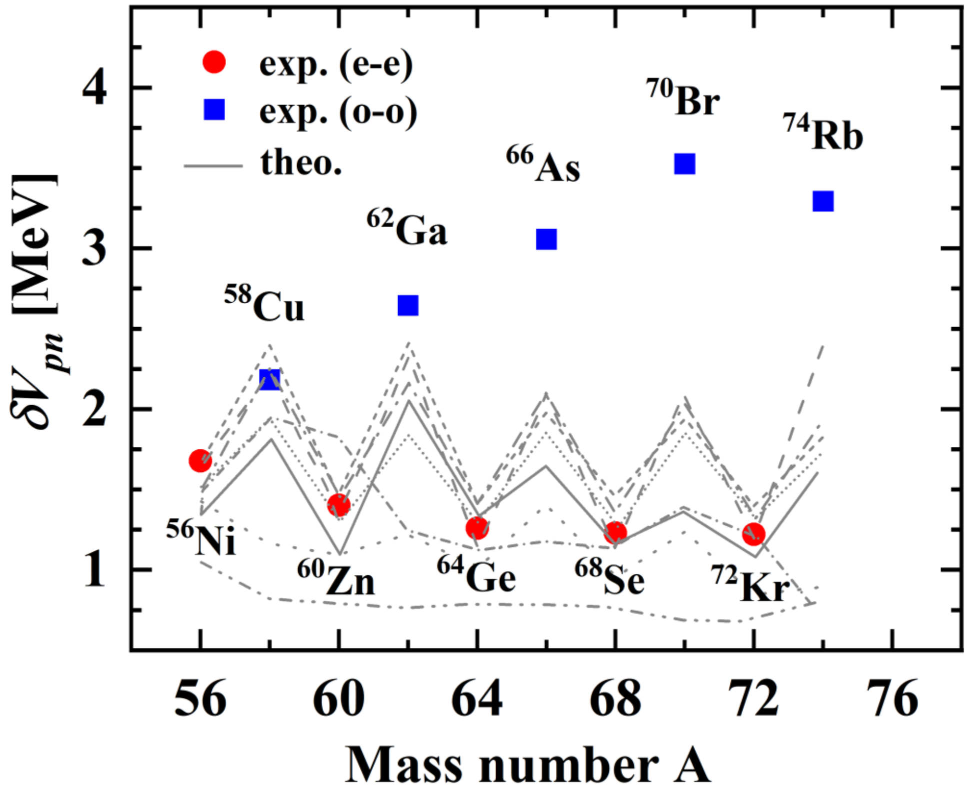

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Kortelainen et al., PRC 85 (2012) 024304

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Goriely et al., PRC 88 (2013) 061302(R)

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Geng et al., PTP 113 (2005) 785

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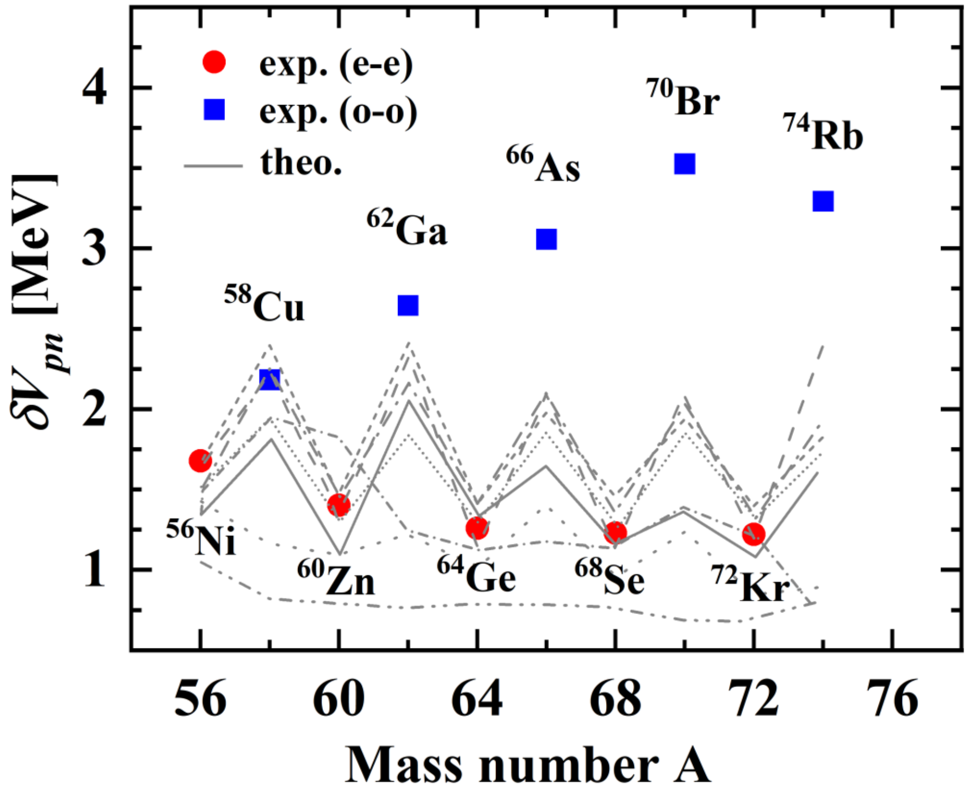

Wang et al., PRL 130 (2023) 192501

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Geng et al., PTP 113 (2005) 785

- What is the missing piece in these models? *maybe pn pairing correlations.*

DFT + Shell-Model-Like Approach (SLAP)

- The nuclear DFT starts from a universal density functional and has achieved great successes in describing many nuclear phenomena.

  a promising framework to microscopicly consider pn pairing correlations

  Vautherin, Brink, PRC 5 (1972) 626
  Meng (Ed.), *Relativistic Density Functional for Nuclear Structure* (2016)

- Shell-Model-Like Approach *an important tool to treat pairing correlations*

  Yang, Zeng, Acta Physica Sinica 20 (1964) 846; Zeng, Cheng, NPA 405 (1983) 1
  Volya et al., PLB 509 (2001) 37

  - Advantages:
    - good particle number; **Particle-Number-Conserving Method**
    - treating the blocking effects exactly. **Exact Pairing Method**
  - Different Versions: *only nn and pp pairing correlations considered*
    - Cranking Nilsson Model + SLAP
      Zeng et al., PRC 50 (1994) 1388; He et al., NPA 817 (2009) 45; Zhang et al., NPA 816 (2009) 19
    - Nonrelativistic DFTs + SLAP
      Pillet et al., NPA 697 (2002) 141; Liang et al., PRC 92 (2015) 064325
    - Relativistic DFTs (RDFT) + SLAP
      Meng et al., FPC 1 (2006) 38; WYP, Meng, PLB 841 (2023) 137923; Xu et al., PRL 133 (2024) 022501
    - ...

This work

a) A new version of RDFT + SLAP is developed, which allows a microscopic treatment of the *nn*, *pp* and *pn* pairing correlations simultaneously.

b) The developed approach is applied to investigate the abnormal δV_{pn} bifurcation for the $N = Z$ nuclei from Ni to Rb.

RDFT-SLAP: Many-body Hamiltonian

In RDFT-SLAP, the many-body Hamiltonian reads

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{pair}}.$$

- One-body part: $\hat{H}_0 = \sum_{k>0} \left[\varepsilon_k^{\pi} (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) + \varepsilon_k^{\nu} (b_k^\dagger b_k + b_{\bar{k}}^\dagger b_{\bar{k}}) \right].$

  $\varepsilon_k^{\pi(\nu)}$: single-proton (neutron) energies obtained from the Dirac equation,

$$[-\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta(m + S) + V]\psi_k = \varepsilon_k \psi_k.$$

$$S(\boldsymbol{r}) = \alpha_S \rho_S + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \Delta\rho_S,$$

$$V(\boldsymbol{r}) = \alpha_V \rho_V + \gamma_V \rho_V^3 + \delta_V \Delta\rho_V + \tau_3 \alpha_{TV} \rho_{TV} + \tau_3 \delta_{TV} \Delta\rho_{TV} + e\frac{1-\tau_3}{2} A^0.$$

- Pairing part: $\hat{H}_{\text{pair}} = \sum_{T_z=0,\pm1} \hat{H}_{\text{pair}}^{T_z}, \qquad \hat{H}_{\text{pair}}^{T_z} = -G \sum_{k,k'>0}^{k\neq k'} P_{k,T_z}^\dagger P_{k',T_z}.$

  The *pp*, *pn* and *nn* pair creation operators are respectively:

$$P_{k,-1}^\dagger = a_k^\dagger a_{\bar{k}}^\dagger, \qquad P_{k,0}^\dagger = \frac{1}{\sqrt{2}}(b_k^\dagger a_{\bar{k}}^\dagger + a_k^\dagger b_{\bar{k}}^\dagger), \qquad P_{k,1}^\dagger = b_k^\dagger b_{\bar{k}}^\dagger.$$

RDFT-SLAP: Many-body Wave function

- Nuclear many-body wave functions:

$$|\Psi\rangle = \sum_{i,\{s_k\}} C_i^{\{s_k\}} \left|\mathrm{MPC}_i^{\{s_k\}}\right\rangle .$$

$C_i^{\{s_k\}}$: expansion coefficients

$$|\mathrm{MPC}_i^{\{s_k\}}\rangle = |l_1 l_2 \cdots l_N m_1 m_2 \cdots m_Z\rangle = b_{l_1}^\dagger b_{l_2}^\dagger \cdots b_{l_N}^\dagger a_{m_1}^\dagger a_{m_2}^\dagger \cdots a_{m_Z}^\dagger |0\rangle$$

- Occupation probabilities for the single-particle states:

$$n_k^{\pi(\nu)} = \sum_{i,\{s_k\}} |C_i^{\{s_k\}}|^2 P_i^{k,\pi(\nu)}, \qquad P_i^{k,\pi(\nu)} = \begin{cases} 1, & \psi_k^{\pi(\nu)} \text{ is occupied in } \mathrm{MPC}_i^{\{s_k\}}, \\ 0, & \text{otherwise.} \end{cases}$$

- Nucleon densities calculated by the occupation probabilities:

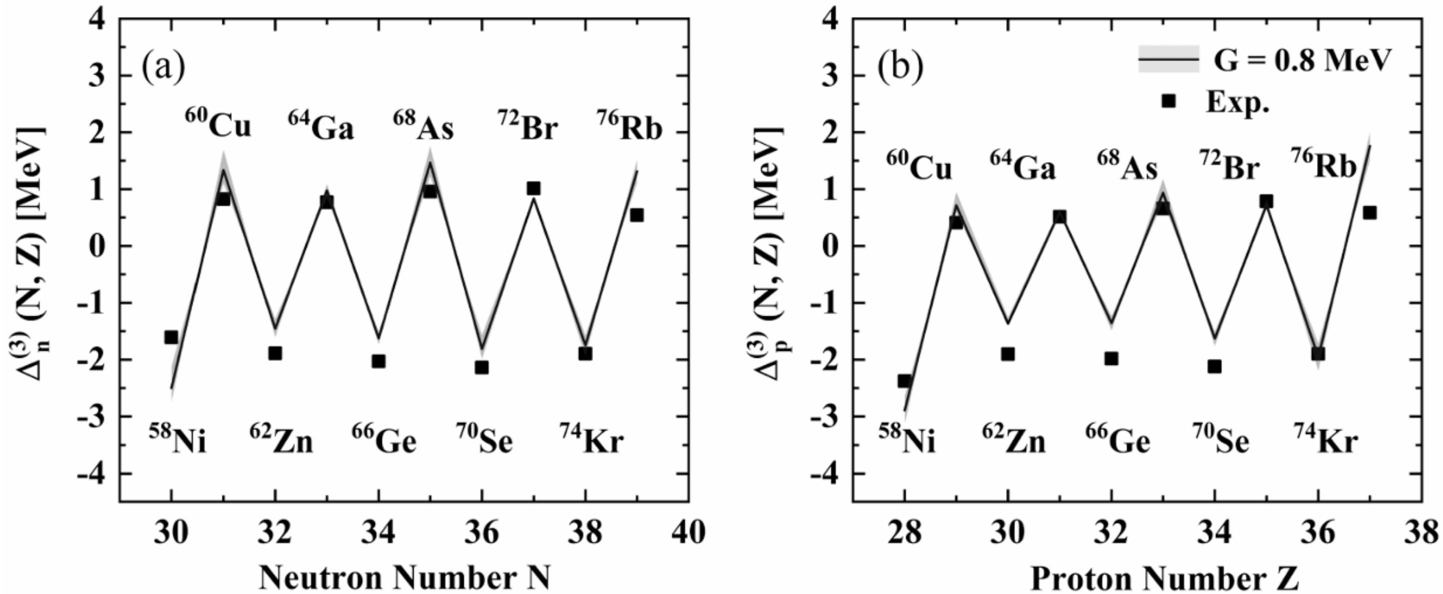
$$\rho_S(\boldsymbol{r}) = \sum_k n_k \bar{\psi}_k(\boldsymbol{r}) \psi_k(\boldsymbol{r}), \qquad \rho_V(\boldsymbol{r}) = \sum_k n_k \psi_k^\dagger(\boldsymbol{r}) \psi_k(\boldsymbol{r}),$$

$$\rho_{TV}(\boldsymbol{r}) = \sum_k n_k \psi_k^\dagger(\boldsymbol{r}) \tau_3 \psi_k(\boldsymbol{r}), \qquad \rho_c(\boldsymbol{r}) = \sum_k n_k \psi_k^\dagger(\boldsymbol{r}) \frac{1-\tau_3}{2} \psi_k(\boldsymbol{r}).$$

which in turn determines *S* and *V* in the Dirac equation.

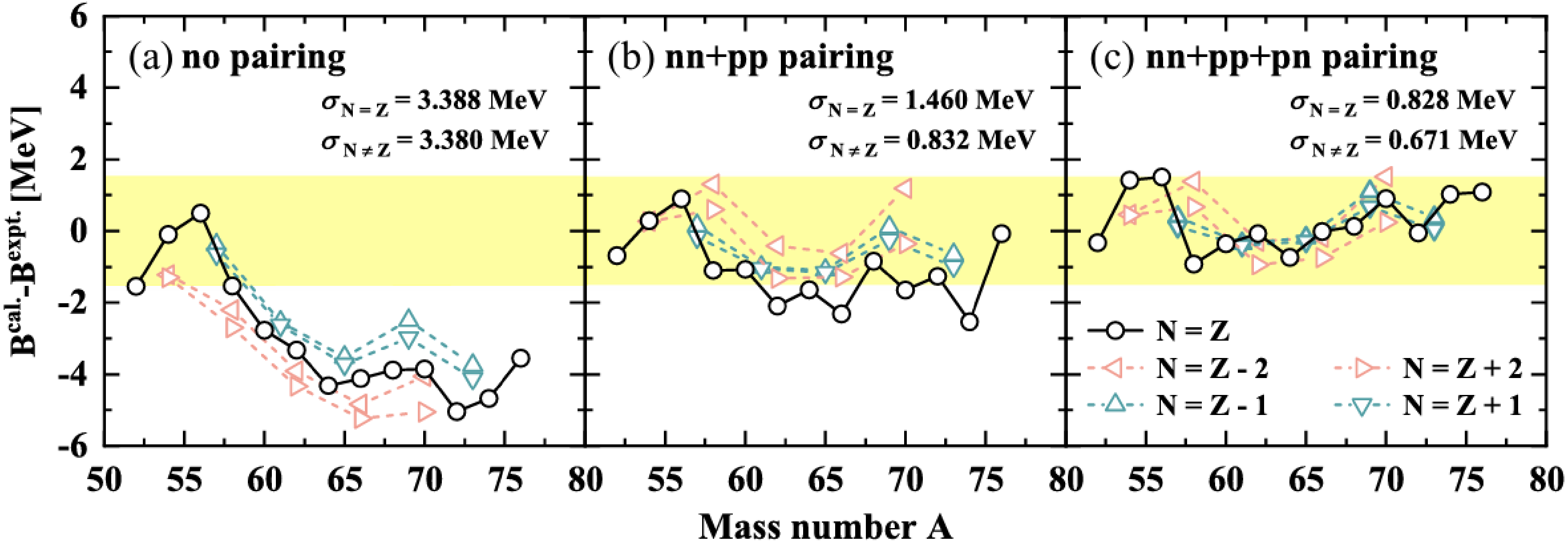
Numerical Details

- Density functional： PC-PK1 P. W. Zhao *et al.*, PRC 82 (2010) 054319
- Major shells of the 3DHO bases： 10
- Energy truncation for MPC space： 16 MeV
- Pairing strength： G = 0.8 MeV



Data from M. Wang *et al.*, CPC 45 (2021) 030003 ; F. G. Kondev *et al.*, CPC 45 (2021) 030001

Descriptions of Binding Energies



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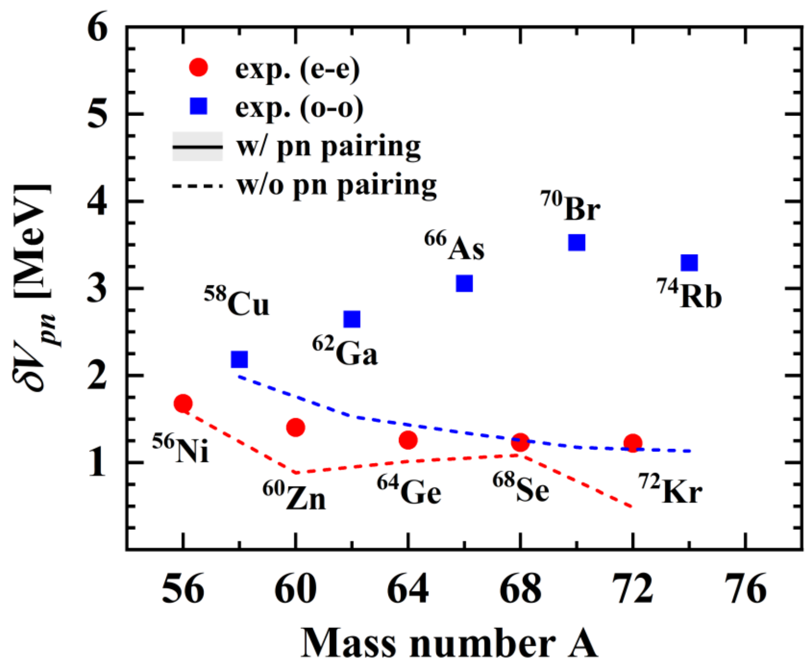
M. Wang et al., PRL 130 (2023) 192501

The pairing correlations are important for these nuclei near the N = Z line, in particular the *pn* pairing correlations.

Interpretation of δV_{pn} bifurcation



$$\delta V_{pn}^{\text{o-o}}(N,Z) = \frac{\partial^2 B}{\partial N \partial Z} = B(N,Z) - B(N-1,Z) - B(N,Z-1) + B(N-1,Z-1)$$

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Van Isacker et al., PRL 74 (1995) 4607

The *pn* pairing correlations would significantly enhance the δV_{pn} for odd-odd $N = Z$ nuclei, and thus result in the δV_{pn} bifurcation.

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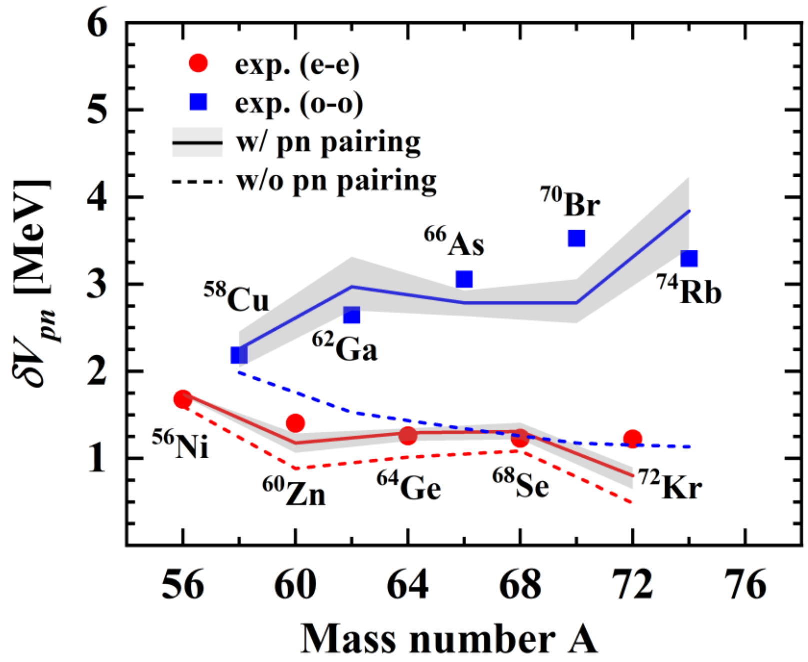

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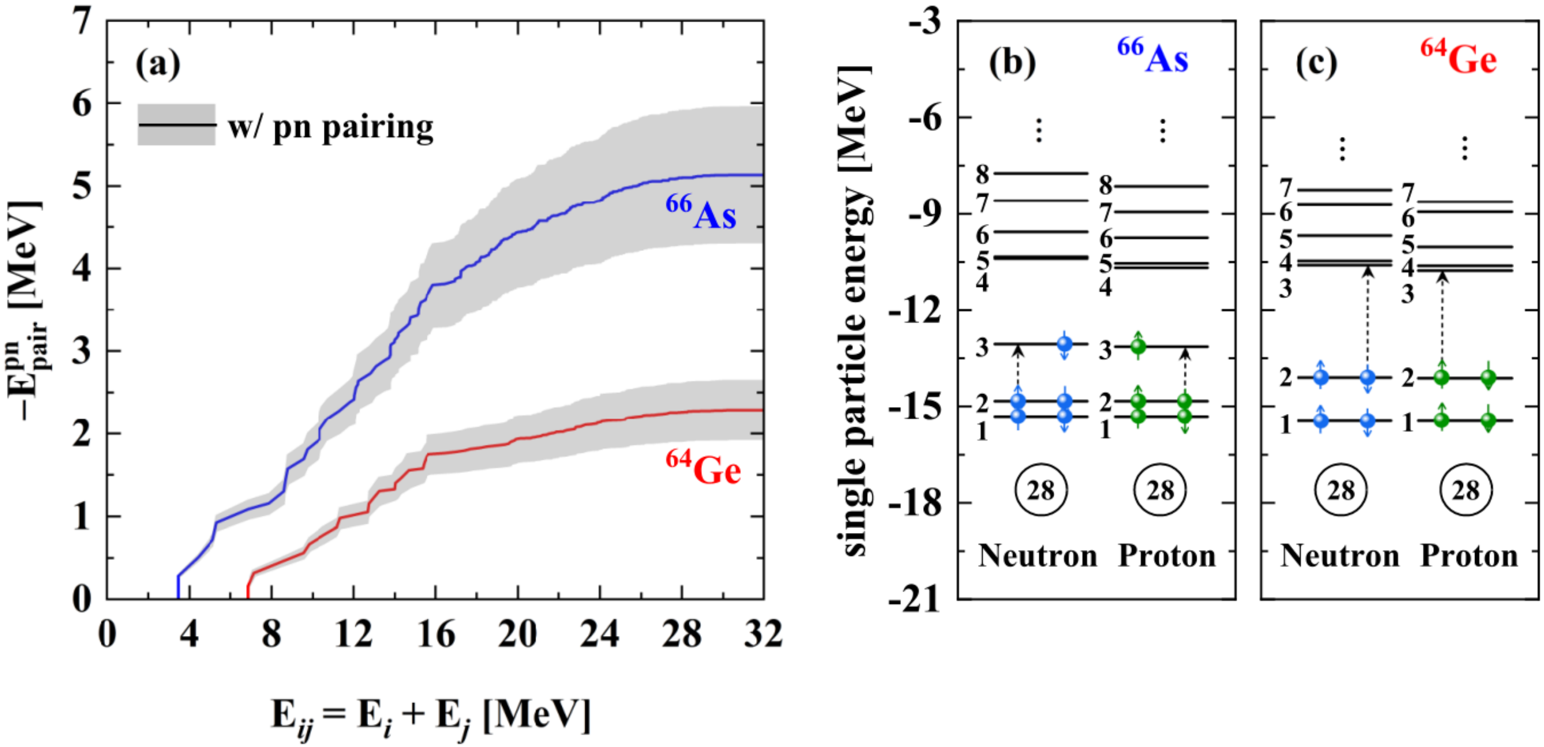
How to understand the *pn* pairing effects on δV_{pn}



$$E^{\rm pn}_{\rm pair} = \langle \Psi | \hat{H}^{T_z=0}_{\rm pair} | \Psi \rangle = \sum_{ij} C_i^* C_j \langle {\rm MPC}_i | \hat{H}^{T_z=0}_{\rm pair} | {\rm MPC}_j \rangle$$

Compared with $^{64}\mathrm{Ge}$, there are more MPCs with low excitation energies contributing nonzero *pn* pairing energy $E^{\rm pn}_{\rm pair}$ for $^{66}\mathrm{As}$.

Summary and Outlook

Summary

RDFT + SLAP calculations with *nn*, *pp* and *pn* pairing correlations:

- provide a good description of the masses for nuclei near $N = Z$ line
- provide an excellent interpretation of the δV_{pn} bifurcation
- reveal a clear signal for the existence of *pn* pairing correlations

Outlook

The newly developed method and its extensions can also be used for:

- δV_{pn} for nuclei in other mass regions
- Rotational properties for $N = Z$ nuclei
- Possible signals of isoscalar pairing correlations

Thank you for your attention!