Calculating nucleon-pair gaps, math and drawing

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1 Basic Concepts

Denote atomic mass, atomic nucleus mass, neutron mass, proton mass, electron mass, and mass excess as M_A, M_N, m_n, m_p, m_e and M_{ex} respectively, mass number, neutron number, proton(and so electron) number as A, N, Z, atomic mass unit as amu, electrons and nuclear binding energies as $B_e(Z), B(Z, N)$, according AME2020[WHK+21]

$$B_e(Z) = 14.4381 \times Z^{2.39} + 1.55468^{-6} \times Z^{5.35} eV.$$

We have

$$\begin{aligned} M_N(Z, N) &= M_A(Z, N) - Z \times m_e + B_e(Z) \\ &= A \times amu + M_{ex}(Z, N) - Z \times m_e + B_e(Z). \end{aligned} \tag{1}$$

1.1 Binding energy

The total binding energy of nucleus (Z, N) is defined as

$$\begin{aligned} B(Z, N) &= Z \times m_p + N \times m_n - M_N(Z, N) \\ &= Z \times m_p + N \times m_n - A \times amu - M_{ex}(Z, N) + Z \times m_e - B_e(Z), \end{aligned} \tag{2}$$

it is usually the binding energy per nucleon provided in atomic mass table,

$$B_A(Z, N) = B(Z, N)/A.$$

The binding energy per nucleon for Ca and Sn isotopes provided in AME2020 is showing in Figure 1, the odd-even staggering effect can be observed, the even-N isotopes are more bound than its neighboring odd-N isotopes,

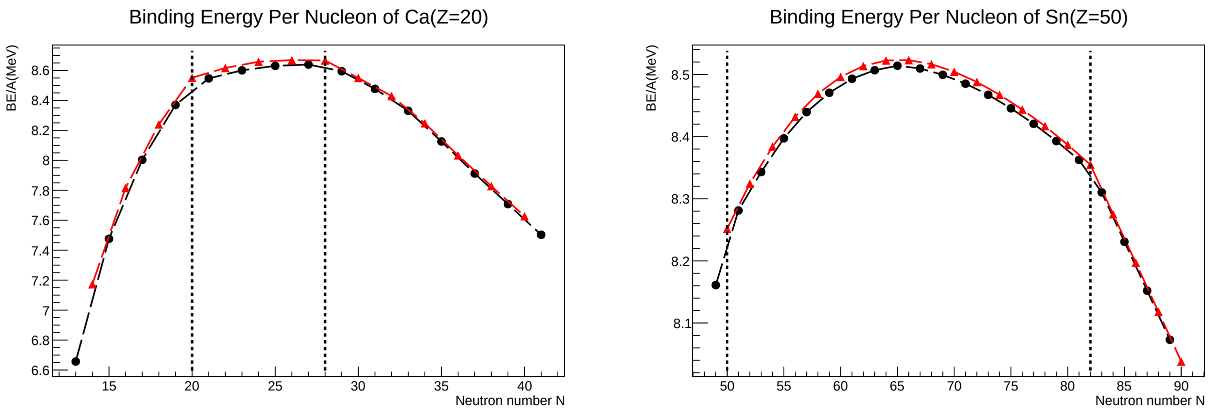
$$B(N_{even}) > \frac{B(N_{even} - 1) + B(N_{even} + 1)}{2},$$

the dashed vertical lines in the figures indicate the positions of magic numbers of neutrons and protons, one can find in the figures that for these nuclei with magic neutron or proton numbers the binding energies are stronger. The same effect can be observed in Figure 2.

The binding energy of isotones of $N = 20, 21, 50, 51$ are presenting in Figure 3 and Figure 4, and the same odd-even staggering effect is existing in such odd-Z isotones.

Across all $Z = const$ isotopes and $N = const$ isotones in the above figures, **the binding energies of even-Z or even-N nuclei are always stronger than that of their neighboring odd-Z or odd-N nuclei**,

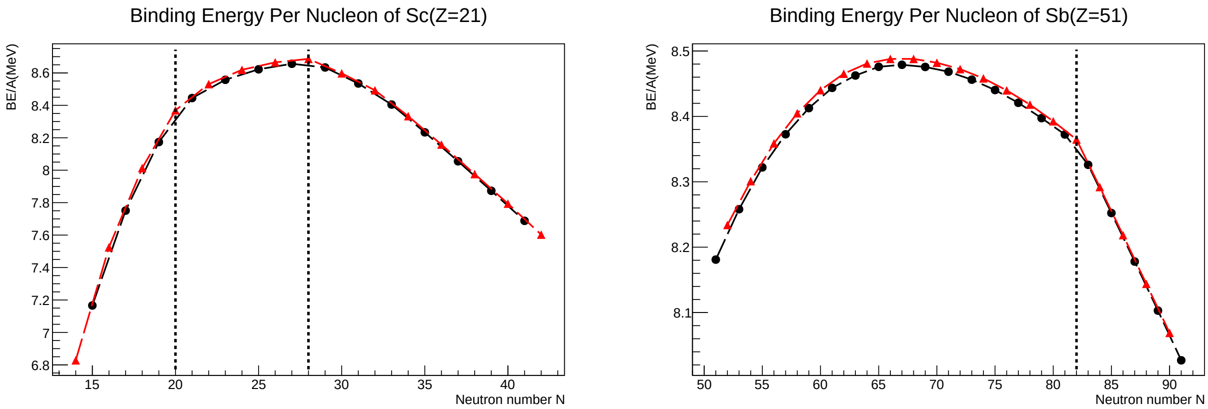
$$B(Z_{even}) > \frac{B(Z_{even} - 1) + B(Z_{even} + 1)}{2}.$$



(a) Calcium isotopes.

(b) Tin isotopes.

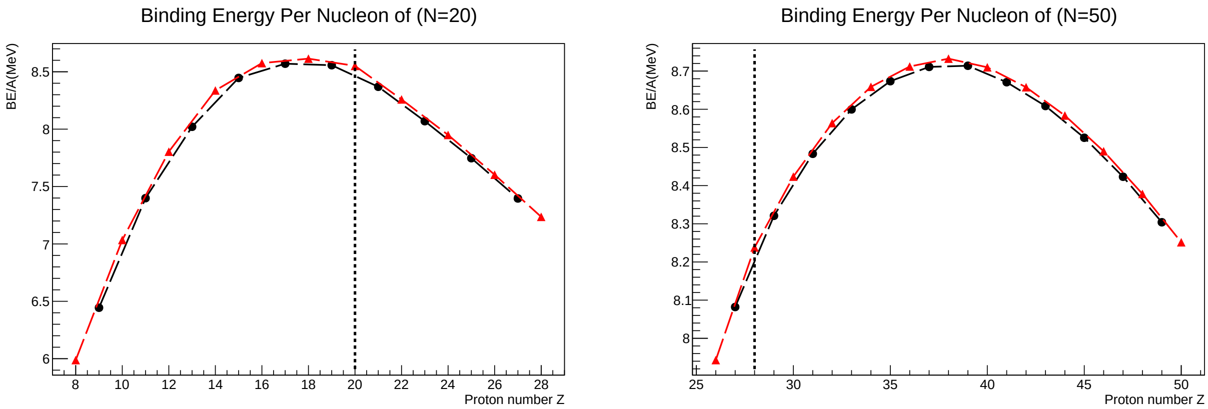
Figure 1: Binding energy per nucleon of calcium, tin isotopes. The red triangles represent even-N, the black dots for odd-N.



(a) Scandium isotopes.

(b) Antimony isotopes.

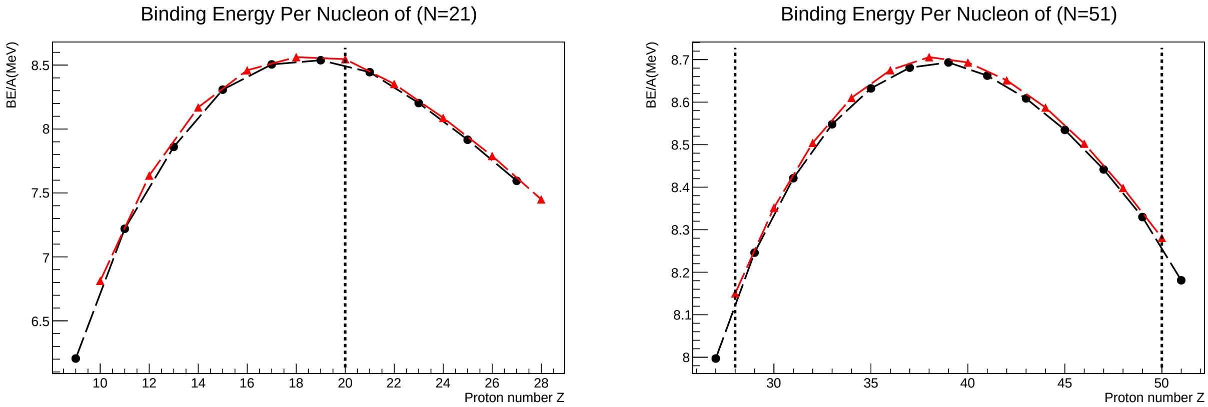
Figure 2: Binding energy of scandium, antimony isotopes.



(a) $N = 20$ isotones.

(b) $N = 50$ isotones.

Figure 3: Binding energy of $N = 20, 50$ isotones.



(a) $N = 21$ isotones.

(b) $N = 51$ isotopes.

Figure 4: Binding energy of $N = 21, 51$ isotones.

1.2 One particle separation energy

The neutron separation energy of nucleus (Z, N) is the energy required to remove a neutron, the neutron is free and the residual nucleus is in its ground state, the amount of the energy

$$\begin{aligned} S_n(Z,N) &= B(Z,N) - B(Z,N-1) \\ &= m_n - 1amu - M_{ex}(Z,N) + M_{ex}(Z,N-1), \end{aligned} \tag{3}$$

the one for proton is

$$\begin{aligned} S_p(Z,N) &= B(Z,N) - B(Z-1,N) \\ &= m_p - 1amu + m_e - M_{ex}(Z,N) - B_e(Z) \\ &+ M_{ex}(Z-1,N) + B_e(Z-1). \end{aligned} \tag{4}$$

Take Ca and Sn isotopes as examples, we get the curves of their one-neutron separation energy and one-proton separation energy vs neutron number N as in Figure 5. It's clear that in Figure 5a and Figure 5b the last neutron in the isotopes with even number of neutrons are more bound, the even-odd staggering (EOS) can be observed, one should realize that for a even-N nucleus to separate a neutron from a nucleus the energy required to overcome the mean field S'_n is not the full story, the residual interaction between two last neutrons Δ_{nn} which is contributing an additional amount of binding energy as well,

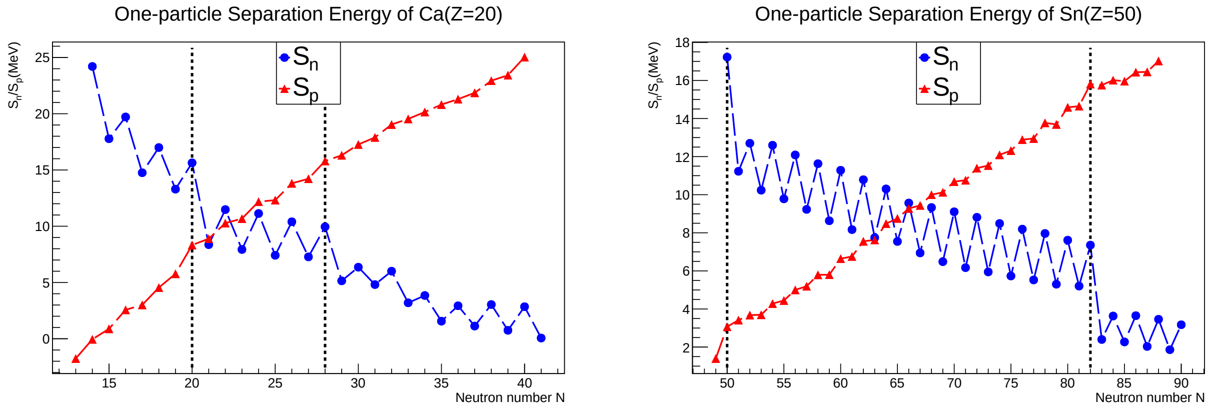
$$S_n(N_{even}) = S'_n(N_{even}) + \Delta_{nn}(N_{even}).$$

While if it's an odd-N nucleus there is no paired last two neutrons, so the Δ_{nn} in last equation just vanishes,

$$S_n(N_{odd}) = S'_n(N_{odd}).$$

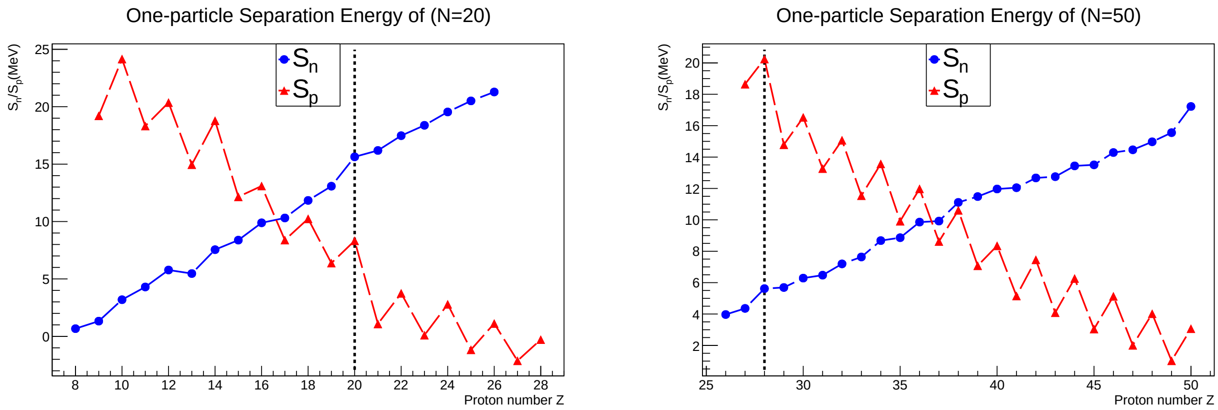
In case of the proton separation, such a staggering can also be noticed while the slope only changes with very small fluctuation compared with that of S_n. The decreasing and increasing tendencies with neutron number of S_n and S_p reflect the increasing richness of neutrons in Ca and Sn, with N increasing the neutron is easier to pick up, and proton is harder to get separated. The rapid drop of S_n at $N = 51, 83$ is the effect of closed magic shell.

In Figure 6a and Figure 6b for $N = 20$ and $N = 50$ isotones the staggering of S_p becomes much more stronger, and it keeps decreasing with proton number, greater drops at the magic proton number $Z = 20, 28$ can be observed.



(a) Calcium isotopes. (b) Tin isotopes.

Figure 5: One particle separation energy of calcium, tin isotopes. The red triangles represent the proton separation energies, the blue dots for neutron separation.



(a) $N = 20$ isotones. (b) $N = 50$ isotones.

Figure 6: One particle separation energy of $N = 20, 50$ isotones.

In case of the odd-Z nuclei in Figure 7, the entire patten does not change so much. The difference is, in Figure 5 where Ca and Sn are even-Z nuclei, data of proton separation energy S_p indicate that the last proton is more bound in even-N isotopes than what it is in odd-N isotopes

$$S_p(Z_{even}, N_{even}) > \frac{S_p(N_{even} - 1) + S_p(N_{even} + 1)}{2},$$

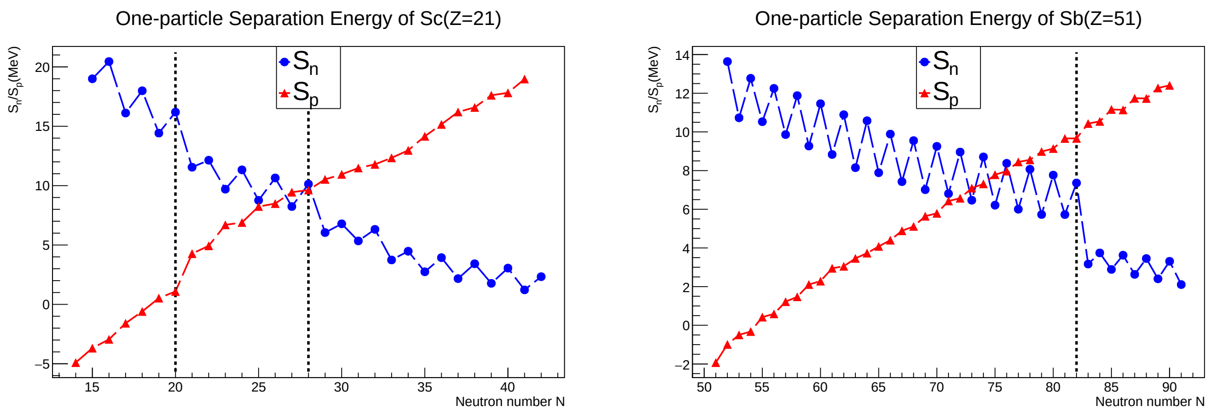
while in odd-Z nuclei, where there is an unpaired proton in isotopes chain, as it's showing in Figure 7, the last unpaired proton is more bound in odd-N isotopes than in their neighboring even-N isotopes

$$S_p(Z_{odd}, N_{odd}) > \frac{S_p(N_{odd} - 1) + S_p(N_{odd} + 1)}{2},$$

this is confusing because we are expecting a loose binding of an unpaired proton, while actually what we got is a tighter binding.

The same situation is happening in Figure 8 for S_n in $N = 21, 51$ isotones compared with Figure 6, the last unpaired neutron of the isotones chain is more bound in the odd-Z isotones than in their neighboring even-N isotones

$$S_n(Z_{odd}, N_{odd}) > \frac{S_n(Z_{odd} - 1) + S_n(Z_{odd} + 1)}{2}$$



(a) Scandium isotopes.

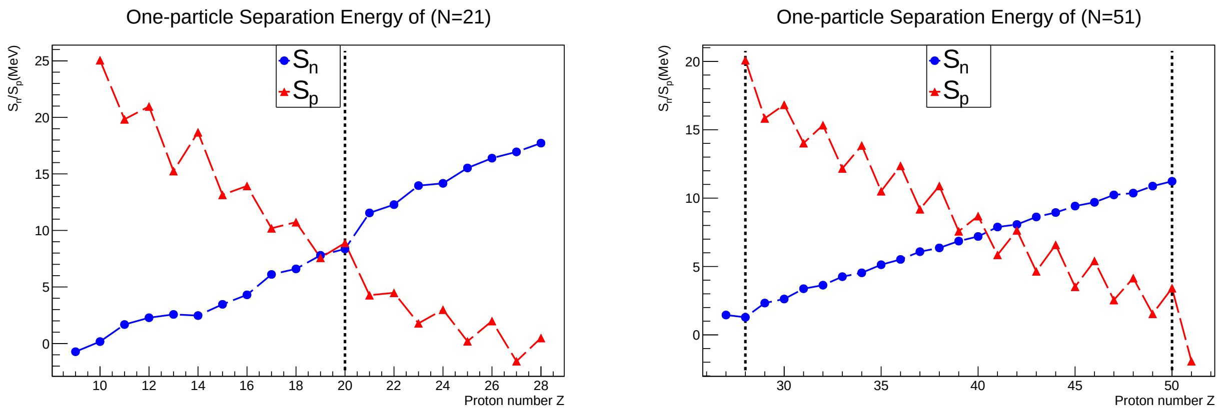
(b) Antimony isotopes.

Figure 7: One particle separation energy of scandium, antimony isotopes.

the relationship holds for every odd-Z isotones, which is in contrary to the fact in $N = 20, 50$ isotones chains

$$S_n(Z_{even}, N_{even}) > \frac{S_n(Z_{even} - 1) + S_n(Z_{even} + 1)}{2}.$$

This may reflect the competition and mutual-exclusion between the interactions of two like-nucleons(Δ_{nn}, Δ_{pp}) and two unlike-nucleons(δ_{np})?.



(a) $N = 21$ isotones.

(b) $N = 51$ isotones.

Figure 8: One particle separation energy of $N = 21, 51$ isotones.

In even-Z isotopes (say all protons are paired) if the last neutron is paired with another neutron, which corresponds to the isotopes with even-N, the extra binding energy would be contributed to the system, it would not in case of odd-N because the last neutron is left alone. In odd-Z isotopes the interaction between the last proton and the last neutron in an odd-N isotope could also makes the system more bound, no such additional binding in even-N isotopes where the last proton is left unpaired. The question is: **can the additional np binding energies in odd-odd nuclei cover the like-nucleon pairing binding energy in neighboring odd-Z even-N nuclei?**

1.3 Two particles separation energy

The two-neutron separation energy is the required energy to remove two neutrons from (Z, N), the amount of the energy

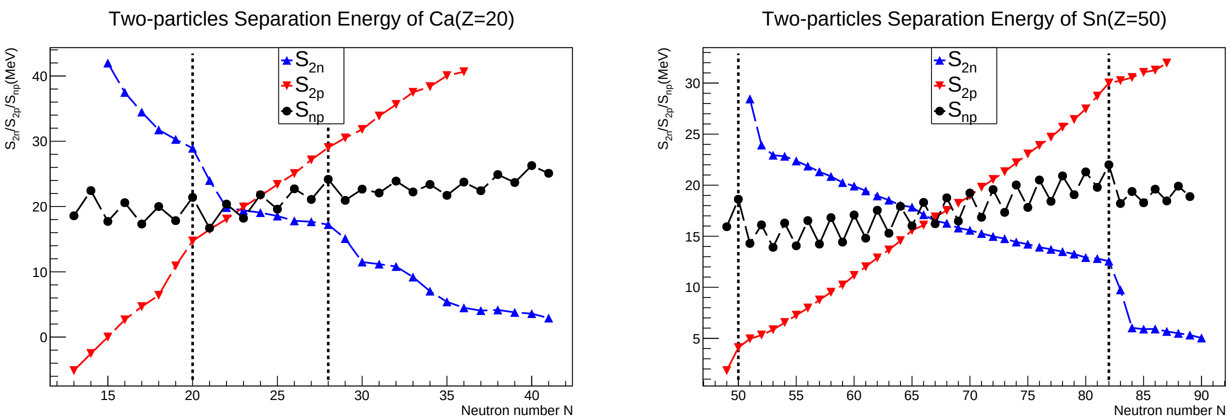
$$\begin{aligned} S_{2n}(Z,N) &= B(Z,N) - B(Z,N-2) \\ &= 2m_n - 2amu - M_{ex}(Z,N) + M_{ex}(Z,N-2), \end{aligned} \tag{5}$$

from the Equation 5 it's clear that the two neutrons separated from the mother nucleus are free neutrons, any kind of interaction energy between two neutrons is destroyed by default, and the daughter nucleus is in its ground state, the actual separation energy would be greater if it's the excited state daughter nucleus is populated.

What if the two-neutrons is still in their bound state?

The separation equation for the two-proton separation is

$$\begin{aligned} S_{2p}(Z,N) &= B(Z,N) - B(Z-2,N) \\ &= 2m_p - 2amu + 2m_e - M_{ex}(Z,N) - B_e(Z) \\ &+ M_{ex}(Z-2,N) + B_e(Z-2). \end{aligned} \tag{6}$$



(a) Calcium isotopes.

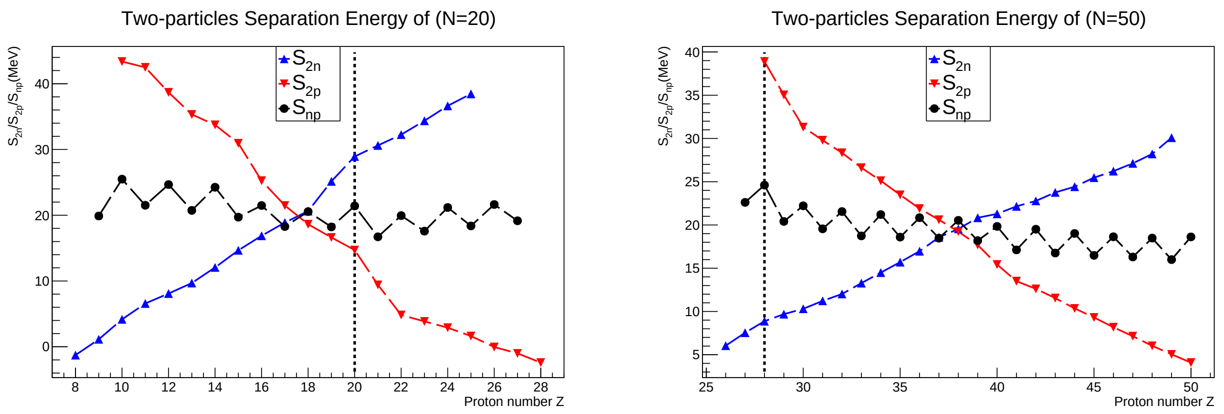
(b) Tin isotopes.

Figure 9: Two particles separation energy of calcium, tin isotopes. The red triangles represent the two-proton separation energies, the blue triangles for two-neutron separation, and black dots are neutron-proton separation energies.

The neutron-proton separation energy is

$$\begin{aligned} S_{np}(Z,N) &= B(Z,N) - B(Z-1,N-1) \\ &= m_p + m_n - 2amu + m_e - M_{ex}(Z,N) - B_e(Z) \\ &+ M_{ex}(Z-1,N-1) + B_e(Z-1). \end{aligned} \tag{7}$$

The data were presented in Figure 9 and Figure 10 for isotopes chains of Ca and Sn, isotones chains of $N = 20, 50$. The magic number effects can be observed, such as the radical drop of S_{2n} of Ca and Sn isotopes at $N = 20, 28, 50, 82$ in Figure 9 and S_{2n} of Sc and Sb isotopes at $N = 20, 28, 82$ in Figure 11, while the strong odd-even staggering for two-neutron separation and two-proton separation energies is found to be canceled, it's easy to understand because for two-neutrons (like-nucleons) separation no matter it's odd-N or even-N an amount of energy Δ_{nn} has to be paid, there is no additional binding energy producing such a fluctuation any more. In case of two unlike-nucleons separation if it's an odd-Z odd-N nucleus there is no Δ_{nn} or Δ_{pp} needs to



(a) $N = 20$ isotones.

(b) $N = 50$ isotones.

Figure 10: Two particles separation energy of $N = 20, 50$ isotones.

break, while for an even-Z even-N nucleus both Δ_{nn} and Δ_{pp} need to break, for odd-even nucleus Δ_{nn} or Δ_{pp} needs to break, and so the EOS manifests itself in neutron-proton separation energy, S_{np}, in both isotope case and isotone case.

In Figure 11 no flip relationship found compared with Figure 9, the relationship

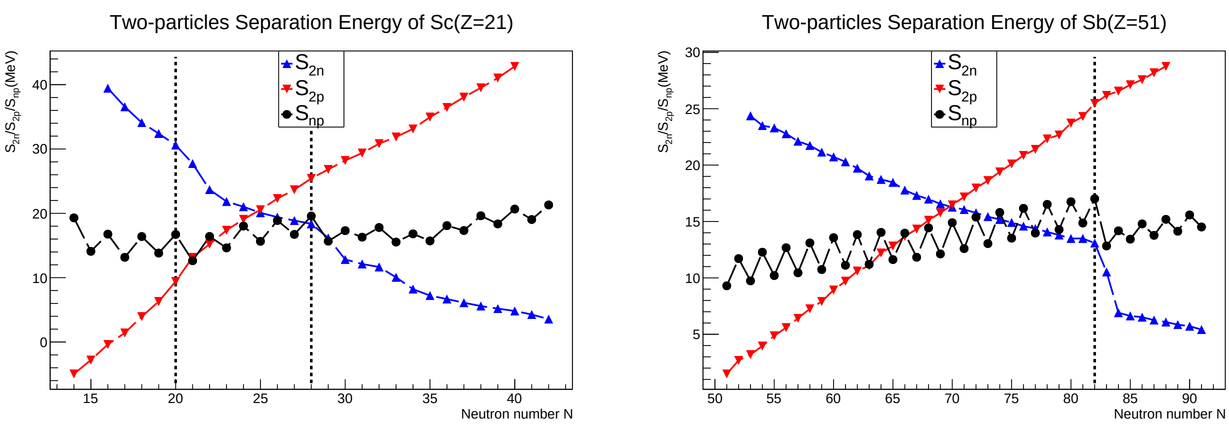
$$S_{np}(N_{even}) > \max[S_{np}(N_{even} - 1), S_{np}(N_{even} + 1)],$$

holds no matter the number of protons is odd or even.

From the data of isotones one can find that

$$S_{np}(Z_{even}) > \max[S_{np}(Z_{even} - 1), S_{np}(Z_{even} + 1)],$$

holds for both odd-N and even-N isotones in Figure 10 and Figure 12.

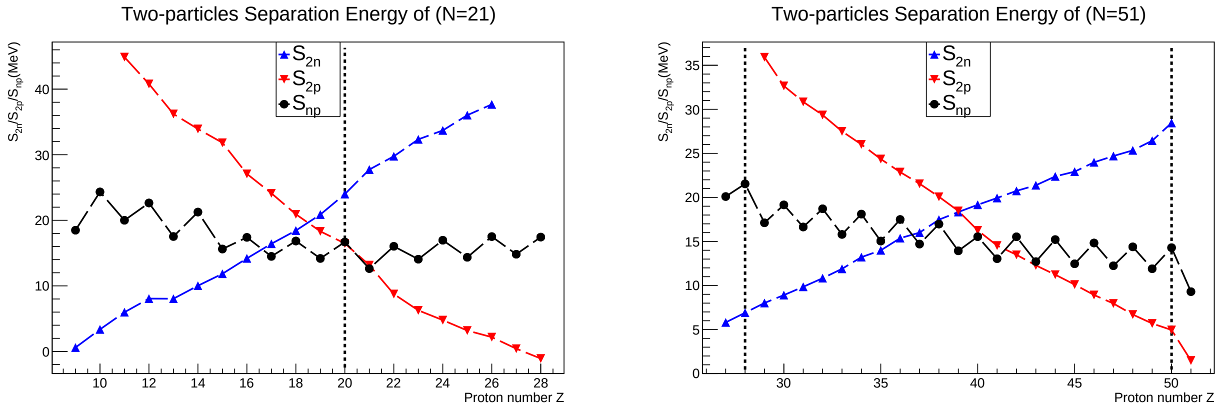


(a) Scandium isotopes.

(b) Antimony isotopes.

Figure 11: Two particles separation energy of scandium, antimony isotopes.

The drop of S_{np} is larger at $N = 50, 82$ than it is at $N = 20$ in Figure 9, and a drop at $N = 82$ in Figure 11b. A large drop of S_{np} at $Z = 28$ can be observed in Figure 10b, and at $Z = 28, 50$ in Figure 12b, indicating a stronger binding effect with the neutron or proton number approaching the number corresponding to the magic shells. Another conclusion is for a heavier system the changing of not just two-neutron separation or two-proton separation but neutron-proton separation is smoother and more continuous, and the drops after magic shells are sharper and more pronounced.



(a) $N = 21$ isotones. (b) $N = 51$ isotones.

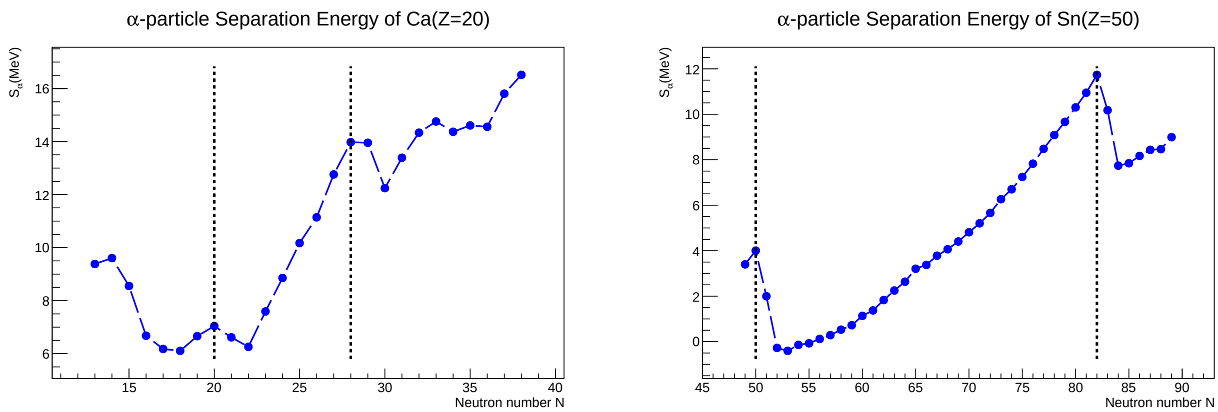
Figure 12: Two particles separation energy of $N = 21, 51$ isotones.

1.4 α particle separation energy

The α particle separation energy is the required energy to remove one α rather than two free protons and two free neutrons from nucleus (Z, N), the amount of the energy,

$$S_\alpha(Z, N) = B(Z, N) - B(Z - 2, N - 2) - B(2, 2), \tag{8}$$

which actually also is Q-value(positive), Q_α. From the Equation 8 it's clear that the four nucleons separated from the mother nucleus are not free but bound in the ground state of α. As it's showing in Figure 13 the α separation energy increases with the neutron number N between two main shells, and a rapid drop follows beyond the magic N number.

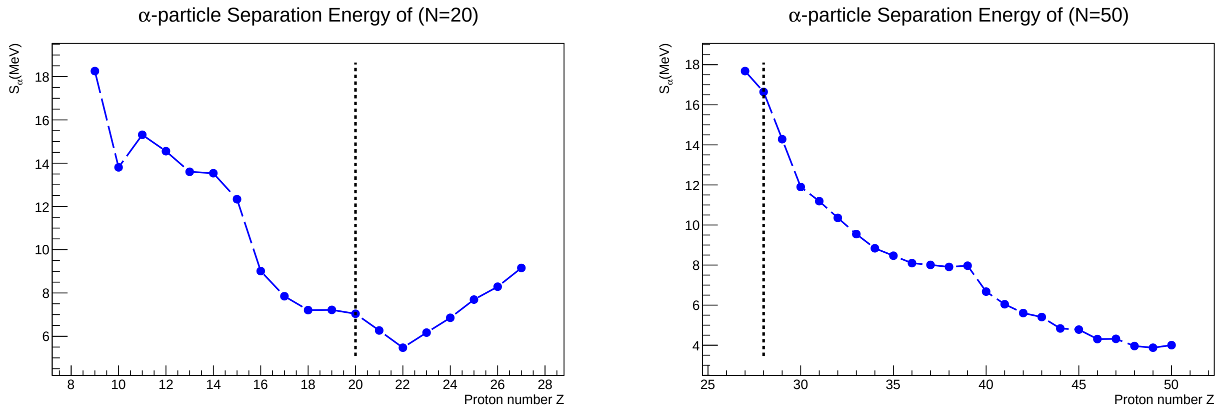


(a) Ca isotopes. (b) Sn isotopes.

Figure 13: One alpha particle separation energy of Ca and Sn isotopes.

In Figure 14b for isotones with $N = 50$ the completely different situation is happening, the separation energy keeps decreasing with proton number Z, the same decline in Figure 14a for isotones with $N = 20$ while there is a turning at $Z = 22$ after which α particle separation becomes harder.

For neutron-rich nuclei it would be easier to separate neutrons and more difficult to separate protons, the increasing in between two shells in Figure 13 means that the separation energy of two-protons increases faster than that to separate two-neutrons, for proton-rich nuclei in Figure 14 the energy decreasing in separating two-protons is faster than the increasing in separating two-neutrons, so the S_α keeps decreasing, which actually confirmed that α is forced to tunnel out the atomic nucleus due to the Column force among protons. In Figure 13 for fixed number of protons, more neutrons more difficult to emit an α, in Figure 14 where $N = const$ more protons easier to separate an α.

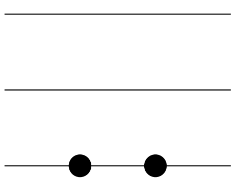


(a) $N = 20$ isotones. (b) $N = 50$ isotones.

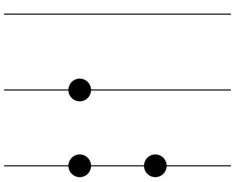
Figure 14: One alpha particle separation energy of $N = 20, 50$ isotones.

2 Pair-correlation Gaps

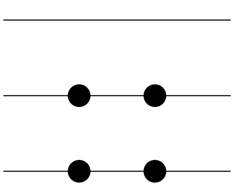
The additional binding energy due to the nucleon-pair correlation Δ can be derived using separation energy. For the unpaired neutron in an odd-N nucleus, say nucleus $(Z, N-1)$, no additional correlation needs to be broken in the process to remove the neutron, while in case of nn pair in an even-N nucleus (Z, N), to separate a neutron from nucleus the pair correlation between two neutrons has to be broken.



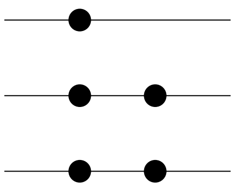
(a) $(Z, N-2)$



(b) $(Z, N-1)$, unpaired last neutron.



(c) (Z, N), paired last neutrons.



(d) $(Z, N+1)$, unpaired last neutron.

Figure 15: Two levels schematics of unoccupied, unpaired and paired neutrons.

Assuming a simplified two-level picture of three neighboring nuclei, $N-2$, $N-1$ and N, $N-2$ taken as the inert core, the rest two with one and two neutrons at the outer shell respectively.

The energy $S_n(Z,N-1)$ should differ from that of (Z,N) by the correlation energy

$$\begin{aligned}\Delta_{nn}(Z,N) &= S_n(Z,N) - S_n(Z,N-1)\\ &= B(Z,N) - 2B(Z,N-1) + B(Z,N-2)\\ &= 2S_n(Z,N) - S_{2n}(Z,N),\end{aligned} \tag{9}$$

Equation 9 was name three-point formula because there are binding energies of three nuclei are taking into account, for a better average S'_n evaluation, four-point (nuclei) formula is recommended[ISTV17].

$$\Delta_{nn}(Z,N) = \frac{2S_n(Z,N) - S_n(Z,N+1) - S_n(Z,N-1)}{2}. \tag{10}$$

There is a five-point formula[MN88],

$$\Delta_{nn}(Z,N) = \frac{3S_n(Z,N+1) - 3S_n(Z,N) + S_n(Z,N-1) - S_n(Z,N+2)}{8}. \tag{11}$$

The calculations of the nn, pp, np pair indicators have been performed using all known nuclides in Figure 16, Figure 17, Figure 18.

In Figure 16 the clear leaps of the gaps at the magic number of neutrons $N = 20, 50, 82, 126$ show the additional binding energy, with N increasing in a main shell the gap continues to be larger and peaks about at the middle of the shell then decreases, it's clear that the odd-Z even-N nuclei has the smaller binding energy compared with the test 3 kinds of pairs systematically.

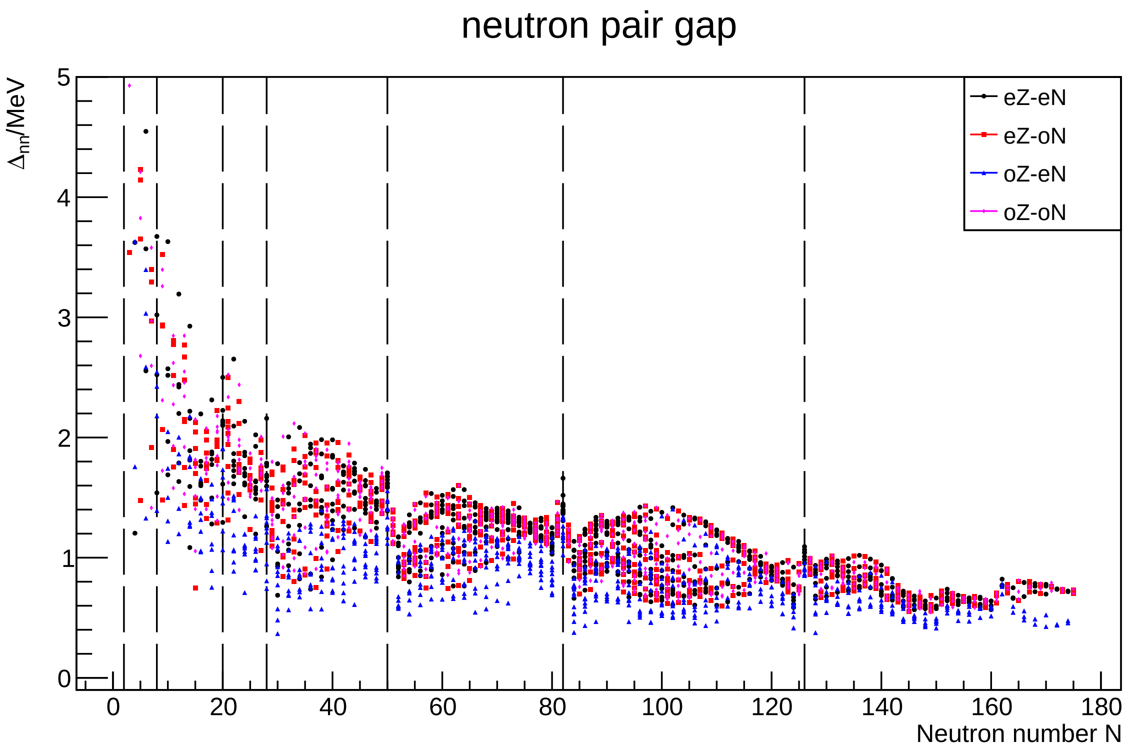


Figure 16: Neutron-neutron pair gaps of all nuclides.

In Figure 18 for *pp* gaps there is no such difference can be found among different sorts of nuclei.

The calculation for the Ca and Sn isotopes chain in Figure 19,

The calculation for the $N = 20, 50$ isotones chains in Figure 20,

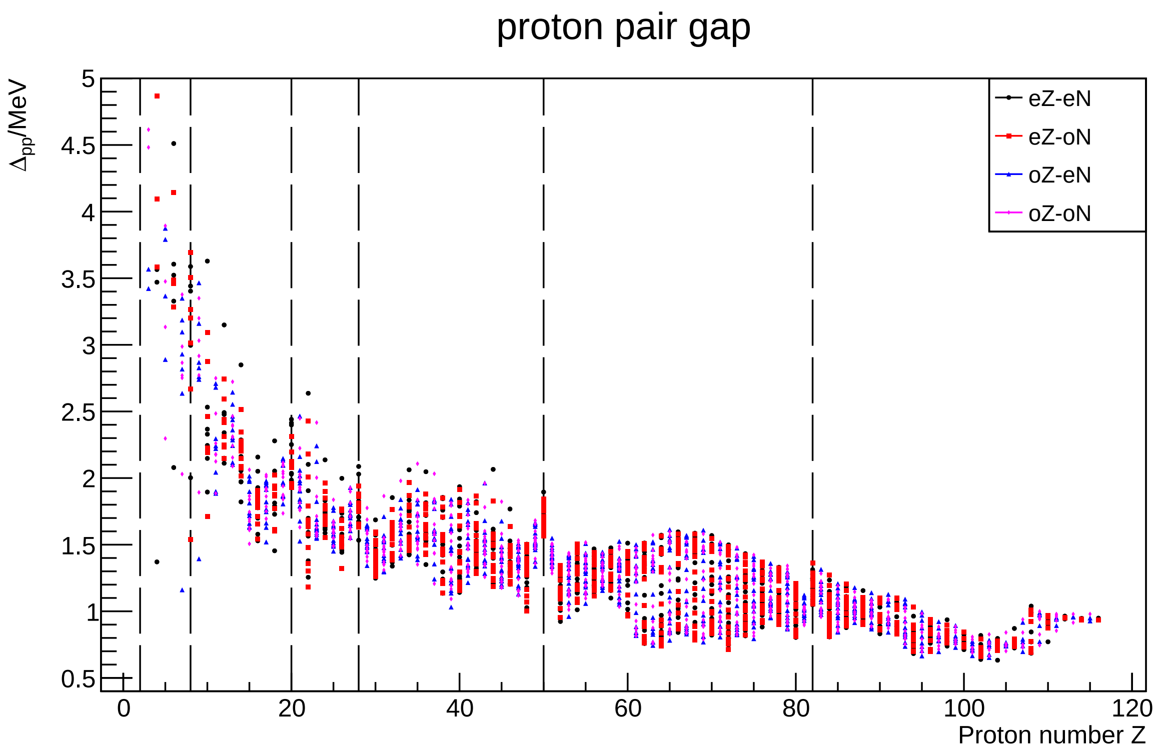


Figure 17: Proton-proton pair gaps of all nuclides.

The calculation for the $N - Z = 0, 20$ isodiaphers chains in Figure 21 and Figure 22,

For the $N = Z$ nuclei the nn and pp pairs share almost the same curve, no matter it's an odd-odd or even-even nucleus. The np gaps of odd-odd and even-even nuclei differ a lot in $A < 20$ region, while the difference shrinks in heavier region. In summary the gaps decrease with nucleon number increasing.

References

[ISTV17] B. S. Ishkhanov, S. V. Sidorov, T. Yu. Tretyakova, and E. V. Vladimirova. Mass differences and neutron pairing in ca, sn and pb isotopes. *Chinese Physics C*, 41(9):094101, sep 2017.

[MN88] David G. Madland and J.Rayford Nix. New model of the average neutron and proton pairing gaps. *Nuclear Physics A*, 476(1):1–38, 1988.

[WHK+21] Meng Wang, W.J. Huang, F.G. Kondev, G. Audi, and S. Naimi. The ame 2020 atomic mass evaluation (ii). tables, graphs and references*. *Chinese Physics C*, 45(3):030003, mar 2021.

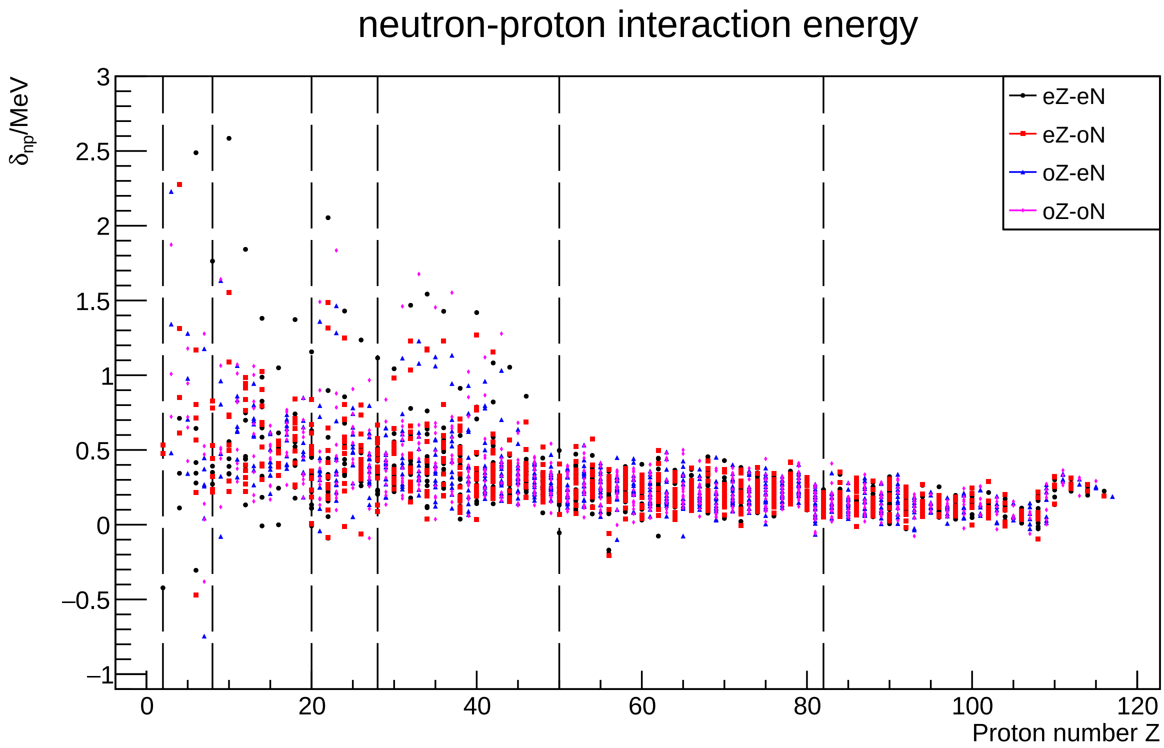
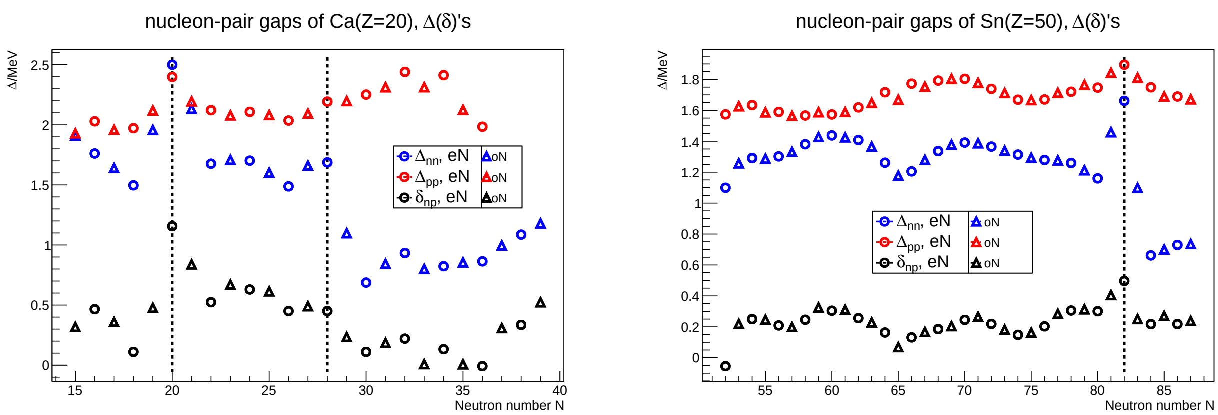


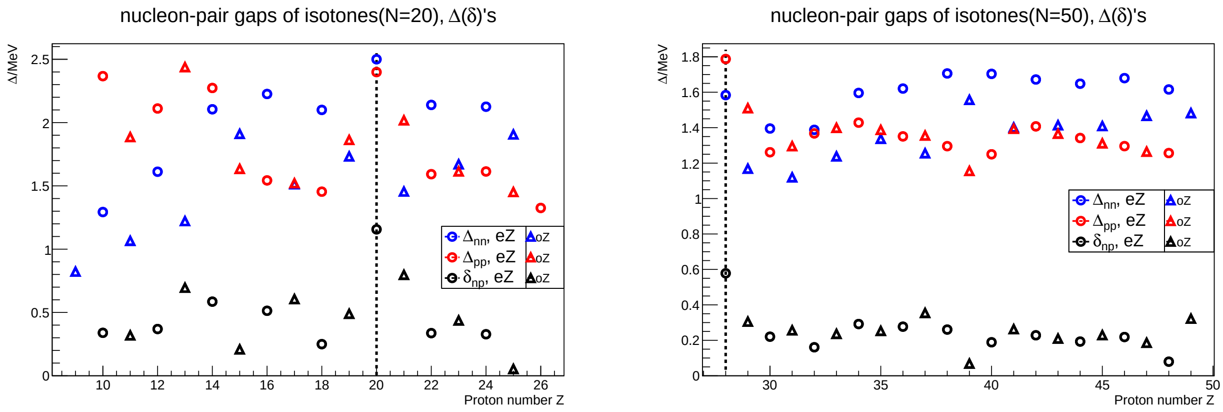
Figure 18: Neutron-proton pair gaps of all nuclides.



(a) Ca isotopes.

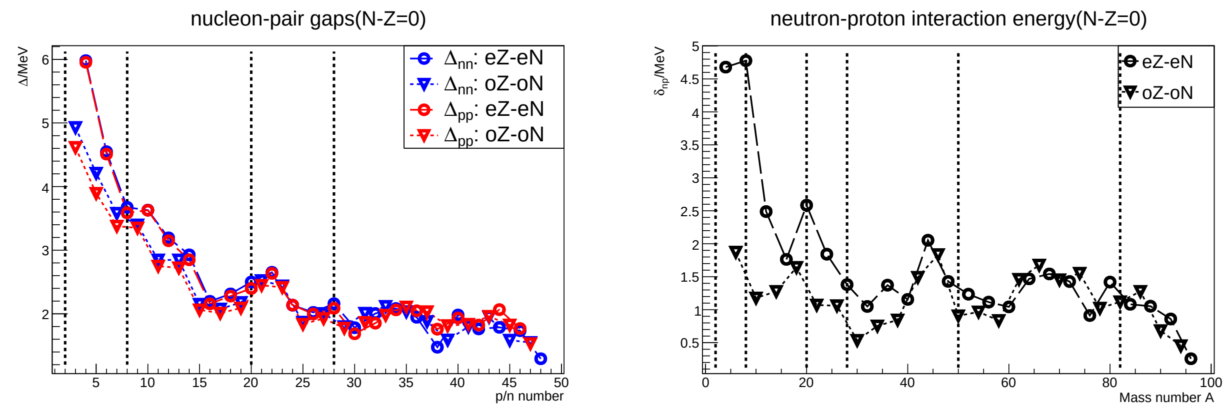
(b) Sn isotopes.

Figure 19: Nucleon-pair gaps of Ca and Sn isotopes.



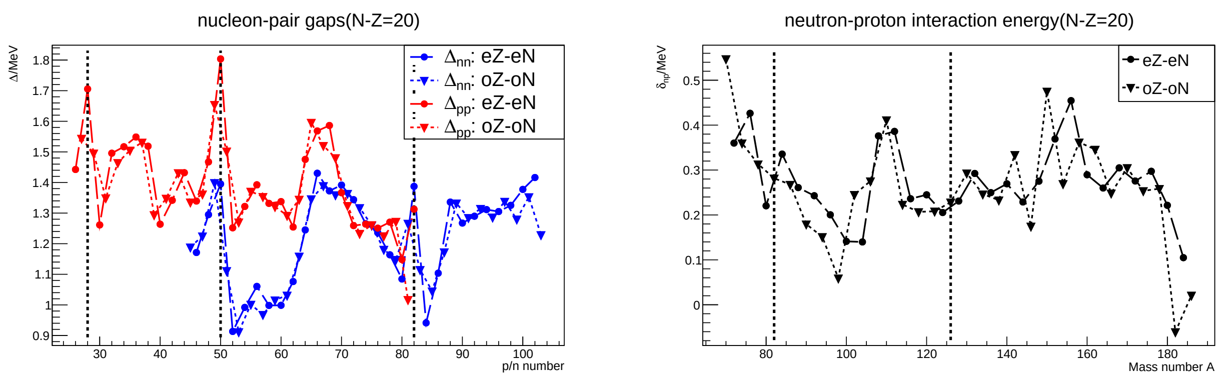
(a) $N = 20$ isotones. (b) $N = 50$ isotones.

Figure 20: Nucleon-pair gaps of $N = 20, 50$ isotones.



(a) $N - Z = 0$ isodiaphers. (b) $N - Z = 0$ isodiaphers.

Figure 21: Nucleon-pair gaps of $N = Z$ isodiaphers.



(a) $N - Z = 20$ isodiaphers. (b) $N - Z = 20$ isodiaphers.

Figure 22: Nucleon-pair gaps of $N - Z = 20$ isodiaphers.