Correlation of Empirical Proton-Neutron Interactions with Growth Rates of Collectivity and DFT Calculations

R.B. Cakirli

[1] Department of Physics, University of Istanbul, Istanbul, Turkey
[2] A.W. Wright Nuclear Structure Laboratory, Yale University, New Haven, CT, 06520, USA

Abstract. Proton neutron interactions give information about configuration mixing, collectivity and deformation in nuclei. Empirical p-n interactions in terms between the last proton(s) and last neutron(s) can be obtained from double differences of binding energies. We will discuss an interpretation with a simple shell model for both closed shell and deformed nuclei, as well as a relation between p-n interaction strengths and the growth rates of collectivity. We will also present results of recent calculations using the nuclear density functional theory.

1 Introduction

Understanding the proton-neutron (p-n) interactions is a fundamental a keystone for the structure of nuclei. There have been many studies of the p-n interaction for years [1–6], and with them the evolution of structure can be explained in terms of, for example, development of configuration mixing, onset of collectivity, deformation in nuclei, phase/shape transitions and magic numbers.

For many-body systems, binding energies reflect the interactions. The sum of all nucleonic interactions is given by nuclear binding energies. Differences of masses give separation energies which highlight shell structure and phase transitions clearly.

Double differences of masses isolate specific classes of interactions and an interaction between the last 2 proton(s) and last 2 neutron(s) which is called as $\delta \mathrm{V}_{pn}$ is given by

$$\begin{aligned} \delta V_{pn}(Z,N) = \frac{1}{4}\,[\{B(Z,N) - B(Z,N-2)\} \\ - \{B(Z-2,N) - B(Z-2,N-2)\}] \end{aligned} \tag{1}$$

Equation 1, for $\delta \mathrm{V}_{pn}$, has 4 binding energies. If there are 4 experimental binding energies, it is possible to extract $\delta \mathrm{V}_{pn}$ experimentally. The first study of $\delta \mathrm{V}_{pn}$ was done by J.Y.Zhang et al., in 1989 [7]. After 2003 mass evaluation [8], new extracted $\delta \mathrm{V}_{pn}$ values were published [9, 10].

$\delta \mathrm{V}_{pn}$ can often be understood in terms of shell structure, depending on the orbits of the last 2 protons and last 2 neutrons in a nucleus. As known, a normal shell

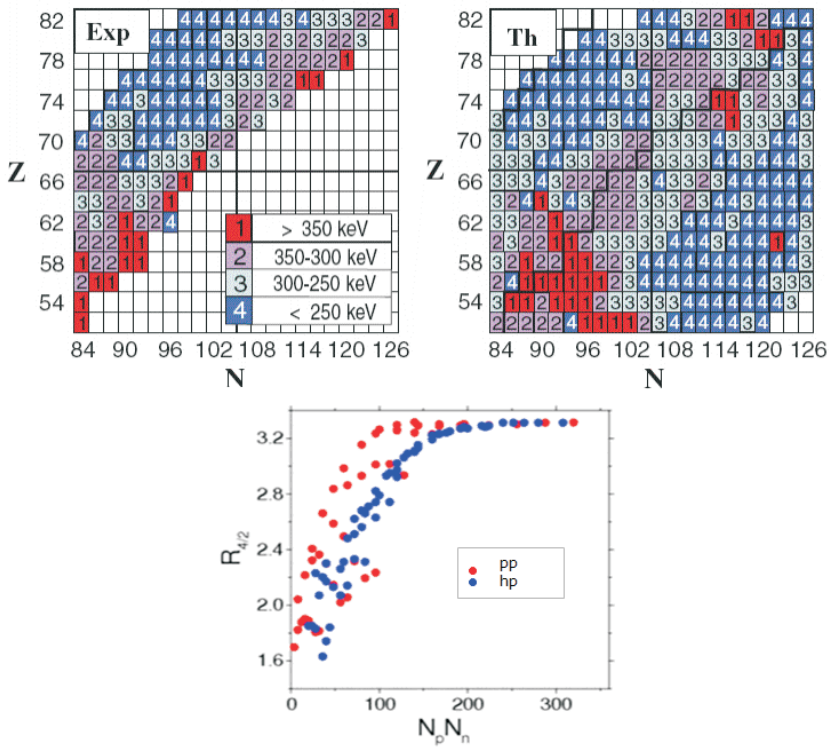

Figure 1. (Top): Empirical and theoretical δV_{pn} results for Z=50-82 and N=82-126 region. (Bottom): $R_{4/2}$ values in the Z=50-82 and N=82-126 region against N_pN_n.

in heavy nuclei begins with high j angular momentum, low n principal quantum number and it ends with low j and high n (for the normal parity orbits). If the protons and neutrons are filling just above a closed shell (for example above 50 and 82, respectively), protons and neutrons will fill orbits that have similar j and n quantum numbers and so we expect a large p-n interaction. However, if the protons and neutrons are filling dissimilar orbits, (that is one of them may fill an orbit above a closed shell and the other one can fill an orbit below a closed shell), we expect a small interaction. Using experimental binding energies, the extracted δV_{pn} values show this idea (Fig. 1(top) of Ref. [9]).

Figure 1 (top) shows experimental and the DFT results (see discussion below) for 50-82 proton and 82-126 neutron shells in a color coded form. The theoretical results will be explained below but notice here that they are similar to the experimental results. Note also that the proton-neutron interaction is stronger in the lower left quadrant, (particle-particle, pp), in Fig.1 (top), and also collectivity (as measured by $R_{4/2}$) grows faster (red points in Fig. 1 (bottom)) in the lower left quadrant than in the upper left quadrant (particle-hole, hp). The upper left quadrant corresponds to smaller p-n interactions with a slower growth of collectivity (blue points

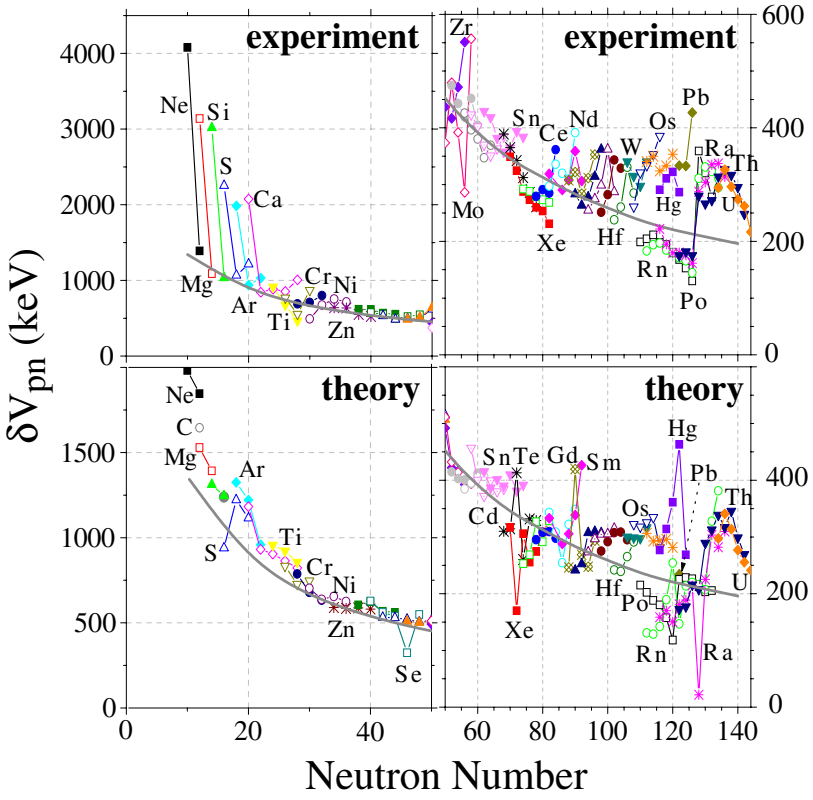

Figure 2. Experimental and theoretical δV_{pn} results for stable nuclei using the SkP functional. (based on Ref. [13])

in Fig. 1 (bottom)). This is the ***first*** direct empirical correlation between p-n interaction strengths and growth rates of collectivity [11].

Theoretical understanding of δV_{pn} is prediction of nuclear masses. Any microscopic calculation should satisfy certain requirements. Of course, it should be based on a solid theoretical approach. Moreover, it should be general so that its predictions are not just limited to known nuclei but so that it can be used to give predictions for unknown mass regions. Lastly, since nuclei have a large variety of structures and shapes, it should be general enough to account for many different classes of collective and intrinsic structure. The Density Functional Theory (DFT) [12] satisfies these requirements and so offers a good testing ground for δV_{pn}. The DFT calculations we present are discussed in Ref. [13] where it is pointed out that they use a self-consistent Hartree-Fock Bogoliubov approach in which pairing is carried out using the Lipkin-Nogami formalism, after which exact particle number projection defines a given nucleus. Several functionals were used and tested, inparticular SkP [14] and SLy4 [15].

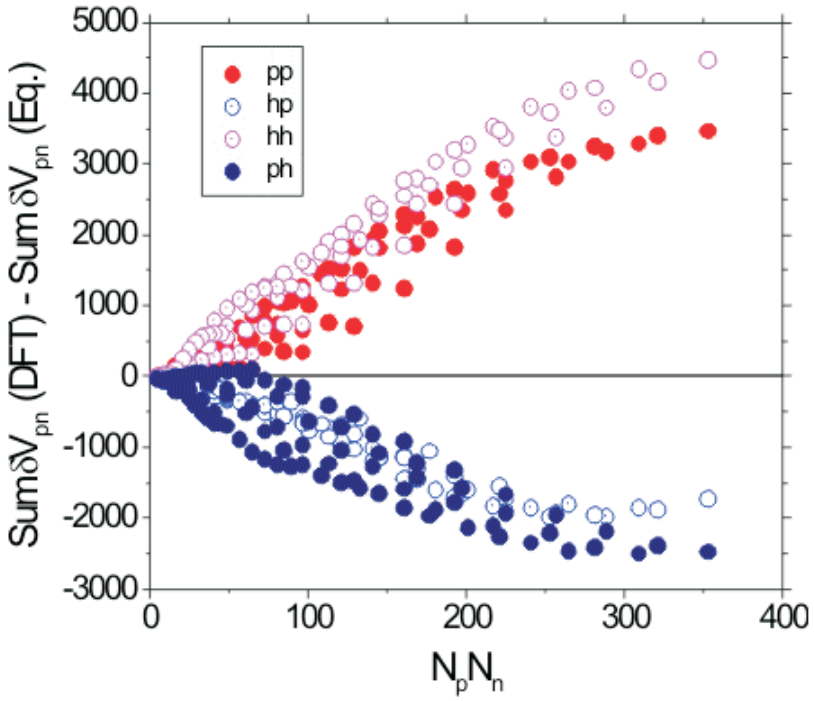

Figure 3. Sum δV_{pn} difference between DFT and Eq. 2 (see text) results against N_pN_n for Z=50-82, N=82-126 region in terms of particle(p) and hole(h).

As mentioned above, Fig. 1 shows experimental and the DFT results for the 50-82 proton and 82-126 neutron shells. If we think in terms of fractional filling of the proton and neutron shells, we can imagine a diagonal line from left bottom to right top: Then we see *reddish* colors along this diagonal more (large δV_{pn} results which is expected). There are more *bluish* colors (lower δV_{pn} results which is expected again) as we go further away from the diagonal line.

DFT calculations were performed for 20 major shells. The δV_{pn} calculations for stable nuclei are illustrated in Fig. 2. The overall trend in the data results from the symmetry energy on top of this, there are fluctuations due specifically to the N and Z dependence of the valence p-n interactions, which arise from the shell structure and correlations in the wave functions. We calculated δV_{pn} (symm) for each nucleus from the DFT masses and compared with the experimental values. As seen from Fig. 2, the overall agreements is very good. The DFT calculations are really impressive, they are working very well. Especially for lower right quadrant, it is wonderful to see this because such calculations can be a nice guide for future mass measurements. There are some discrepancies very close to closed shells (Pb for example) octupole region (Ra at N=128-134 for example). More details about the DFT calculations can be seen in Ref. [13].

$$\widetilde{\delta V}_{pn} \approx 2\left(a_{\rm sym} + a_{\rm ssym} A^{-1/3}\right)/A, \quad (2)$$

In order to get a feeling for the total p-n interaction for any nucleus in a major shell region, we also calculated the sum $\delta \mathrm{V}_{pn}$ considering all neutron and proton numbers (not only last 2 protons and neutrons) from the last shell closures. We then subtracted the symmetry energy as discussed in Ref. [13]. This is illustrated in Fig. 3. This result is actually giving only the orbit-dependent part of the proton-neutron interaction because the total sum $\delta \mathrm{V}_{pn}$ minus the symmetry energy gives specifically the part of the p-n interaction resulting from the overlap between orbitals. Therefore, Fig. 3 should be only overlap part. As can be seen, the hh and pp regions are similar to each other and the hp and ph regions are similar but we see that the hh and pp are larger than the hp and ph regions. This is consistent with our earlier ideas above about the overlaps of the wave functions and the general filling pattern of orbits in heavy nuclei..

DFT is a realistic calculation to produce $\delta \mathrm{V}_{pn}$. We also tried a very simple toy model using a zero-range δ force including spin exchange for the rare earth nuclei [16]. For those calculations, the interaction of the last proton and the last neutron, both occupying Nilsson orbits was calculated using a standard expression for Nilsson wave function in a spherical basis. We obtained very nice results with such a simple interpretation (see Fig. 4 and 5 for Ref. [16]) in the rare earth nuclei, but similar results in the actinides did not reproduce the data [17]. This suggests that a simple approach with Nilsson model wave functions is not generally adequate, pointing to the need for more realsitic calculations such as provided by the DFT.

Acknowledgments

I would like to thank R.F. Casten for his tremendous help and support. I also would like to thank W. Nazarewicz and, M. Stoitsov so much for providing us useful calculations. For our $\delta \mathrm{V}_{pn}$ studies, D.S. Brenner cannot be forgotten and also Y.Oktem and, R.J.Casperson.

Work was supported by the U.S. DOE Grant No. DE-F602-91-ER-40609.

References

1. J.-Y. Zhang, R.F. Casten, and D.S. Brenner, *Phys. Lett.* **B227**, 1 (1989).
2. D.S. Brenner, *et al.*, *Phys. Lett.* **B243**, 1 (1990).
3. P. Van Isacker, D.D. Warner, and D.S. Brenner, *Phys. Rev. Lett.* **74**, 4607 (1995).
4. I. Talmi *Rev. Mod. Phys.* **34**, 704 (1962).
5. K. Heyde, *et al.*, *Phys. Lett.* **155B**, 303 (1985).
6. P. Federman and S. Pittel, *Phys. Lett.* **69B**, 385 (1977) ; *Phys. Lett.* **B77**, 29 (1978)
7. J.-Y. Zhang et al., in *Proceedings of the International Conference on Contemporary Topics in Nuclear Structure Physics Cocoyoc, Mexico, 1988, Book of Abstracts* (unpublished), p. 109.

8. G. Audi, A.H. Wapstra and C. Thibault, *Nucl. Phy.* **A729**, 337 (2003).
9. R.B. Cakirli, D.S. Brenner, R.F. Casten and E.A. Millman, *Phys. Rev. Lett.* **94** , 092501 (2005).
10. D.S. Brenner, R.B. Cakirli and R.F. Casten, *Phys. Rev.* **C**, 034315 (2006).
11. R.B. Cakirli, R.F. Casten *Phys. Rev. Lett.* **96**, 132501 (2006).
12. W. Kohn and L.J. Sham, *Phys. Rev.* **140**, A1133 (1965).
13. M. Stoitsov, R.B. Cakirli, R.F. Casten, W. Nazarewicz and W. Satula, *Phys. Rev. Lett.* **98**, 132502 (2007).
14. J. Dobaczewski, H. Flocard, and J. Treiner, *Nucl. Phys. A* **422**, 103 (1984).
15. E. Chabanat et al., *Nucl. Phys. A* **635**, 231 (1998).
16. Y. Oktem, R.B. Cakirli, R.F. Casten,R.J. Casperson, and D.S. Brenner *Phys. Rev. C* **74**, 027304 (2006).
17. Y. Oktem, priviate communication.