Empirical Proton-Neutron Interactions and Nuclear Density Functional Theory: Global, Regional and Local Comparisons

M. Stoitsov1–3, R.B. Cakirli4,5, R.F. Casten4, W. Nazarewicz1,2,6, W. Satula6

1Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA
2Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
3Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
4Wright Nuclear Structure Laboratory, Yale University, New Haven, CT 06520, USA
5Department of Physics, University of Istanbul, Istanbul, Turkey and 
6Institute of Theoretical Physics, Warsaw University, Warsaw, Poland

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Calculations of nuclear masses, using nuclear density functional theory, are presented for even-even nuclei spanning the nuclear chart. The resulting binding energy differences can be interpreted in terms of valence proton-neutron interactions. These are compared globally, regionally, and locally with empirical values. Overall, excellent agreement is obtained. Discrepancies highlight neglected degrees of freedom and can point to improved density functionals.

As with other many-body systems, the structure of the atomic nucleus depends on the interactions of its constituents, protons and neutrons. These interactions, reflecting the strong and Coulomb forces, and the Pauli Principle, are complex. Nevertheless, their understanding is critical to interpreting nuclear structure and its evolution with $N$ and $Z$. Similar issues arise in other finite complex systems, such as nanostructures, and there is increasing overlap in the theoretical tools applied. In nuclei, where two kinds of fermions come into play, the proton-neutron (p-n) interaction plays the key role in the development of long-range collective correlations, including non-spherical shapes. Due to the shell structure of nuclei, p-n interactions of the valence (open shell) nucleons are the most important.

Since nuclear masses embody the sum of all nucleonic interactions, they provide a laboratory in which it is possible to isolate and extract specific interactions using appropriate mass differences $\delta V_{pn}$. In particular, the average interaction of the last two protons with the last two neutrons in an even-even nucleus is given by the following double difference of binding energies $\delta V_{pn}(Z, N)$:

$$\delta V_{pn}(Z, N) = \frac{1}{4} \left[ (B(Z, N) - B(Z, N - 2)) - (B(Z - 2, N) - B(Z - 2, N - 2)) \right] \quad (1)$$

With the 2003 mass evaluation $M$, it became possible to evaluate a much larger set of $\delta V_{pn}$ values. These have revealed striking bifurcations near closed shells and systematic patterns spanning major shells: a correlation between $\delta V_{pn}$ values and growth rates of collectivity; and intriguing patterns in specific regions. While simple calculations with schematic zero-range interactions give reasonable results in the deformed rare earth nuclei, they fail completely in the actinides. Clearly, a more sophisticated approach is needed.

The indicator involves masses of four neighboring even-even nuclei. Theoretical understanding of the behavior of $\delta V_{pn}$ throughout the whole nuclear chart thus calls for an approach that is capable of predicting nuclear masses with arbitrary $Z, N$ values. Such an approach must fulfill several strict requirements. First, it should be rooted in microscopic theory. Second, it must be general enough to be confidently applied to regions of the nuclear landscape whose properties are largely unknown. Third, it should be capable of handling symmetry-breaking effects resulting in a variety of intrinsic nuclear deformations. These requirements are met by density functional theory (DFT) in the formulation of Kohn and Sham. The main ingredient of the nuclear DFT is the energy density functional describing conditions locally around each nucleon. This can be realized by expressing the functional in terms of local nucleonic densities and currents. The energy functional is augmented by the pairing term describing nuclear superfluidity. When not corrected by additional phenomenological terms, standard functionals, treated self-consistently, reproduce total binding energies with an rms error of 1.5 to 4 MeV. However, they have been successfully tested over the whole nuclear chart for a broad range of phenomena, and usually perform better when applied to energy differences and other global nuclear properties such as radii and nuclear deformations.

As pointed out in Ref. [15], from Eq. (1), $\delta V_{pn}$ approximates the mixed partial derivative

$$\delta V_{pn}(Z, N) \approx \frac{\partial^2 B}{\partial Z \partial N}. \quad (2)$$

For nuclei with an appreciable neutron excess ($T_z > 1$), the average value $\delta \overline{V}_{pn}$ probes the symmetry energy term in the macroscopic mass formula:

$$\delta \overline{V}_{pn} \approx 2 \left( a_{sym} + a_{sym} A^{-1/3} \right) / A, \quad (3)$$
where \( a_{\text{sym}} \) and \( a_{\text{asym}} \) are the symmetry and surface-symmetry energy coefficients, respectively. For nuclei with \( N \sim Z \), \( \delta V_{pn} \) also contains the Wigner energy which can be extracted by taking differences between values of \( \delta V_{pn} \) in neighboring nuclei \[13\]. On top of \( \delta V_{pn} \), detailed fluctuations of \( \delta V_{pn} \) carry important information about shell effects and many-body correlations.

It is the purpose of this Letter to present the first results of large-scale microscopic calculations for \( \delta V_{pn} \) within the DFT framework. Our work demonstrates that, since \( \delta V_{pn} \) is a relative quantity, calculations with realistic functionals can reproduce empirical values \[1\] to significantly better than 100 keV in many mass regions. This is of the same magnitude as local fluctuations in empirical \( \delta V_{pn} \) values. Hence, these calculations can assess the adequacy of currently used energy density functionals and help search for improvements in such aspects as their density dependence and dynamical correlation effects.

The present large-scale calculations of nuclear masses are based on the HFB+THO code described in Ref. \[18\]. Our DFT approach is based on a self-consistent solution of the Hartree-Fock-Bogoliubov equations with an approximate Lipkin-Nogami treatment of pairing followed by an exact particle number projection. Calculations are performed in a transformed harmonic basis spanning 20 major shells. In the particle-hole channel we employed the SkP \[19\] and SLy4 \[20\] Skyrme functionals. The pairing functional corresponds to a density-dependent \( \delta \) interaction of Ref. \[21\]. Unless otherwise indicated, a mixed-type pairing was employed. Overall, over 1000 nuclei were studied. As \( \delta V_{pn} \) corresponds to a second derivative, in order to obtain reliable values, calculations required very high numerical accuracy. In fact, we found out that \( \delta V_{pn} \) provides an excellent check on the precision of calculations. (A similar conclusion was drawn earlier \[8\] in the context of the accuracy of measured masses.)

We first present a global comparison of experimental and theoretical \( \delta V_{pn} \) values in Fig. 1. To accommodate the wide range of \( \delta V_{pn} \) values, while preserving the visibility of the microstructure for heavier nuclei, the panels use different vertical scales. The overall trends in the data are well reproduced by Eq. \[3\] with the SkP values of \( a_{\text{sym}}=30 \) MeV and \( a_{\text{asym}}=-45 \) MeV \[17\]. This confirms empirically the importance of the surface symmetry term. Superposed on this secular decrease there are considerable fluctuations. The most dramatic effect is the empirical singularities in light \( N \sim Z \) nuclei. This is well understood \[8,15\] as resulting in part from \( T=0 \) (p-n) pairing interactions which are not considered in our DFT model. The regional fluctuations on the right seem to have substantial differences between theory and experiment, but a more detailed view provides a more accurate perspective on regions of agreement and regions where the calculations are missing key ingredients.

To pursue this, Fig. 2 shows four isotope chains comprising vibrational systems (Cd), two deformed chains (Ra, U), and proton magic Pb nuclei. The calculations were carried out with the SkP functional with the standard mixed pairing term (SkP) or with the volume pairing (SkPV). For Cd and U, the agreement with experiment is remarkably good for both functionals, and quite acceptable for Ra, generally within a few to 10’s of keV. Given the average mass accuracy of several MeV, this demonstrates a striking ability to probe specific interactions by exploiting the filtering capabilities of mass difference indicators. The Ra-U panels show opposite empirical trends, both well reproduced by the calculations. Yet, there are discrepancies in Ra for \( N=128-134 \) which point to missing physics. Here, an octupole, reflection asymmetric, degree of freedom, not included in the present calculation, plays an important role \[22\]. The Pb nuclei show large discrepancies, reflecting the inadequacy of the current DFT approach for describing strong dynamical changes in “core” structure near magic numbers.

Another interesting feature seen in the SkP and SkPV results of Fig. 2 is that the choice of pairing only weakly affects \( \delta V_{pn} \). This is because, at least for nuclei away from the \( N=Z \) line, the pairing correlation energy can roughly be written as a sum of independent proton (p-p) and neutron (n-n) contributions; hence, the leading components of pairing are expected to be filtered out by the indicator \[23\]. It is instructive to inspect the effectiveness of this filter. Figure 2e shows the differences for the SkP and SkPV calculations in masses, \( \Delta Z_{\text{pn}} \), and \( \delta V_{pn} \). Although the mass differences (BE) range from up to nearly an
tions tested. Figure 3 (top) also shows SkP calculations which also agree better with the data than other interactions. Larger fluctuations than the more robust SkP results, and Skly4 results differ markedly, and in a way rather typically differing by <100 keV), and, for the mixed derivatives δVpn, the differences are essentially zero.

Figure 3 (top) shows three sets of calculations for Er spanning a spherical-deformed transition region. Generally, the SkP and SLy4 functionals (both with the same mixed pairing) reproduce the trends in the data where empirical δVpn values are known (N=84-102), including larger values for the spherical nuclei, a sharp drop in the transition region (N ≈ 90-94), and an increase beyond that. The lower part shows the calculated expectation values of β. These are compared to empirical values of 1/E(21+), which is a useful measure of shape correlation with the moment of inertia. The calculations reproduce the transition region quite well, including the onset of deformation near N=90.92 (perhaps slightly shifted to lower neutron numbers), and its saturation above N=100. Beyond N=102, where no data exist, the SkP and SLy4 results differ markedly, and in a way rather typical for many cases. The SLy4 results often show much larger fluctuations than the more robust SkP results, which also agree better with the data than other interactions tested. Figure 3 (top) also shows SkP calculations where the shape was constrained to a spherical shape. These calculations, of course, are not suitable for transitional or deformed nuclei such as Er and their neighbors, but serve here as a pedagogical benchmark. Excursions above the spherical reference (around the middle of the shell) and below this line (e.g., near N=90) exhibit the effects of shell structure on quadrupole correlations. In this context, it is interesting to recall that the microscopic origin of quadrupole deformations in nuclei can, within the nuclear DFT, be attributed to p-n interactions [23].

The global and local comparisons in Figs. 1-3 are complemented by a regional perspective in Fig. 4. Arguments [2] from generic shell structure can account for the overall systematics. Normal parity orbits fill high-j, low-n orbits early in a major shell, but low-j-high n orbits at the end. Thus one expects the largest δVpn values near the diagonal, where there is similar fractional filling of proton and neutron shells and therefore maximum spatial overlap. At the time of Ref. [5], there were no realistic calculations that could be brought to bear on this empirical phenomenon. However, the power of the nuclear DFT approach is shown by the present calculations which reproduce very well both the general magnitude of δVpn values and their variations across a shell, including larger values near the diagonal. Figure 4 illustrates another point. Overlap arguments again suggest [6] larger empirical δVpn values where protons and neutrons are filling similar quadrants (lower left and upper right) and smaller values in dissimilar regions (upper left). It was speculated [6] that δVpn values would also be small in the currently data-free lower right quadrant. The calculations strikingly confirm this qualitative idea and enhance
the need for new mass measurements in this region.

To conclude, we have presented the first large-scale microscopic DFT calculations of $\delta V_{pn}$ spanning the nuclear chart, comparing the results for different functionals, including different treatments of pairing, and confronting these calculations with empirical results. Overall, the agreement is impressive. This is especially significant since the average error of the calculated binding energies is several MeV. Yet, proton-neutron interaction energies obtained from binding energy differences generally match the data to well under 100 keV and, often, significantly better than that. The agreement is best in the deformed regions where the mean-field theory is expected to capture essential physics. This level of agreement can be exploited to extrapolate to unknown nuclei when three of the four masses needed for a $\delta V_{pn}$ value are known. For example, using the predicted $\delta V_{pn}$ value for $^{238}$U, and the known masses for $^{236}$U and $^{234}$Th, gives a predicted mass excess of -46325 keV for $^{236}$Th. It would be interesting to test this compared to the extrapolation from systematics \cite{audi2003} of -46454 keV. This approach gives useful predictions for ($Z, N-2$) and ($Z-2, N$) nuclei in proton and neutron-rich regions, respectively. Finally, deviations of $\delta V_{pn}$ values do occur, and point to needed improvements in the density functionals, where specific effects or degrees of freedom enter. Example were noted at magic numbers, $N=Z$ nuclei, and in the octupole-correlated Ra region.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{diagram.png}
\caption{Empirical and calculated $\delta V_{pn}$ values for the major shells $Z=50-82$, $N=82-126$, color coded according by magnitude [red for the largest values, blue for the smallest]. (Upper panel taken from Ref. \cite{audi2003}. The zig-zag lines in the theoretical panel enclose nuclei with known empirical $\delta V_{pn}$ values. Four boxes within these lines are empty since some of the nuclei involved are calculated to lie beyond the proton drip line and cannot be calculated reliably by the current DFT model.}
\end{figure}

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