PROCEEDINGS OF SCIENCE

Neuromorphic improvement of the Weizsäecker formula

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Yearly, nuclide mass data is fitted to improved versions of the Bethe-Weizsäecker formula. The present attempt at furthering the precision of this endeavor aims to reach beyond just precision, and obtain predictive capability about the "Stability Island" of nuclides. The method is to perform a fit to a recent improved liquid drop model with isotonic shift. The residuals are then fed to a neural network, with a number of "feature" quantities. The results are then discussed in view of their perspective to predict the "Stability Island".

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1. Introduction

Nuclear reactions providing measurements of masses and a set of other nuclear parameters of nuclei revealed core + skin, or halo characteristics [1]. This lends experimental backing for a nuclear model in which the properties of the nucleus are given by a core + few outer nucleons or holes.

Such a context lends itself possible to model to a certain degree with neuromorphic software in predict the mass defect, although without a physical fundament.

The Bethe-Weizsäecker (BW) mass formula is a satisfactory model for the said core [2]. The idea of a “core” is based on the separation of energy levels. When a substantial gap exists between levels, it is expected that it is too energetically disfavorable for two partici-pant levels to mix, as the repulsion of energy levels shows [3].

Interacting nucleons in an open system observe the same feature, albeit more complex - the transition from isolated to overlapping resonances modifying and separating the width distribu-tions into 2 groups, of super-radiant states and narrow resonances [4].

In this context we can expect that the core does no more than provide a central potential for a 1 halo nucleon, or potential plus additional inter-nucleon interaction term for 2-3-4 nucleon halos (as deuteron halo in 6Li for instance instead of 2 single nucleon states [5]).

The core is composed thus highly stable nucleic configurations, with preferred nucleon numbers, the known magic numbers, delineated by the comparison of experimental binding energies with the Bethe-Weizsäecker mass formula.

The Bethe-Weizsäecker liquid-drop formula can however be improved, before being used as energy model for the core, incorporating isotonic mass shifts [6].

In the liquid drop description of a nucleus of mass number A and atomic number Z, the binding energy is given as:

$$B(A,Z) = a_v A - a_s A^{2/3} - a_c Z(Z-1)/A^{1/3} - a_{sym}(A-2Z)^2/A + \delta$$

with a_v = 15.78 MeV, a_s = 18.34 MeV, a_c = 0.71 MeV, a_{sym} = 23.21 MeV, a_p = 12.0 MeV and the pairing term $\delta = a_p/\sqrt{A}$ (positive for N_{even}-Z_{odd}, negative for N_{odd}-Z_{even} and zero for the rest), as values giving the best fit to the experimental data.

Following the parametrization in [6], to accommodate the date for neutron rich light nuclei away from the valley of stability, we will consider a modified formula:
where $\delta = (1-e^{-A/c})a_p/\sqrt{A}$ (in the same even-odd convention), and c = 30.0, k = 17.0.

$$B(A,Z) = a_v A - a_s A^{2/3} - a_c Z(Z-1)/A^{1/3} - a_{sym}(A-2Z)^2/[(1+e^{-A/k})A] + \delta$$

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1.1 Residuals to experimental data

I have taken the AME2016 data [7] and compared the above considered Bethe-Weizsäecker formula against it.

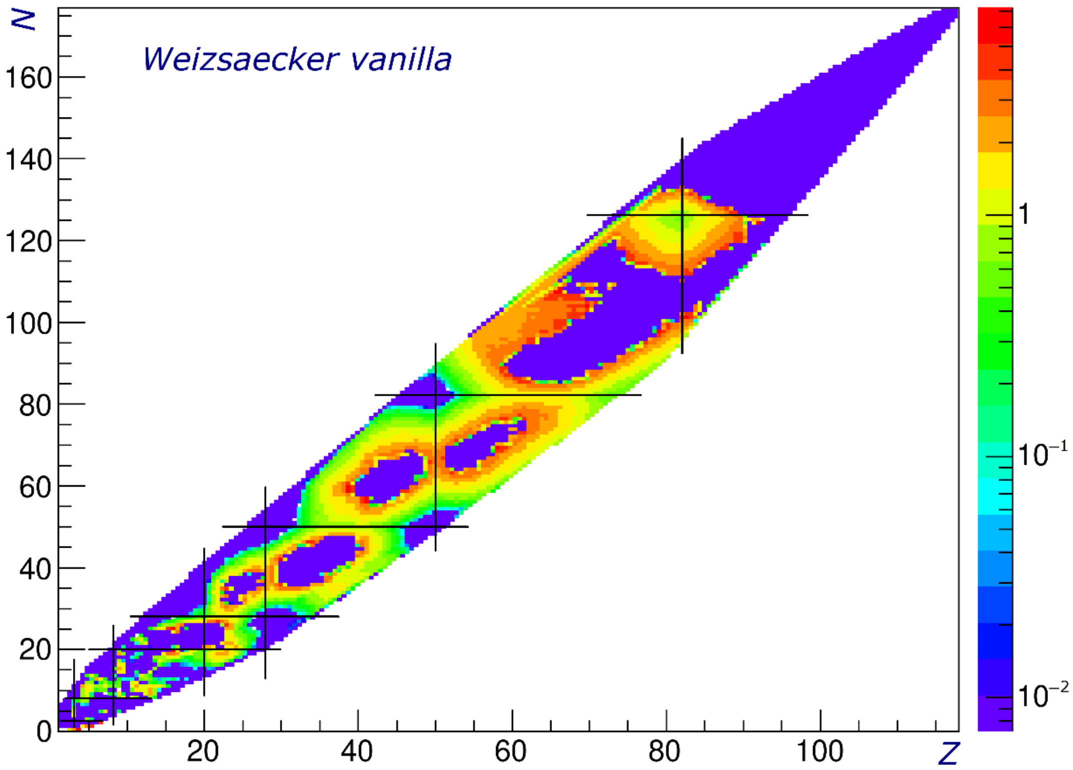

Figure 1: Residuals between experimental data and the Bethe-Weizsaecker liquid drop formula with isotonic shifts. Colors are %'s.

Figure 1 presents the residuals in percentages of the Bethe-Weizsäecker formula relative to the AME2016 data. You can notice excellent agreement (level of 0.01%) in a substantial region of the nuclide chart.

However, as expected, around the magic numbers, the discrepancy widens, reaching levels of 2-3-10%. What is interesting to note is that these discrepancies are not exactly centered on the magic numbers themselves (represented in black lines), rather they are at approximately $\Delta N = \pm 3\text{-}4$, $\Delta Z = \pm 3\text{-}4$.

It is credible that this reveals quantum-rotational bands – not being plausible vibrational modes close to the core's ground state.

It is however less clear that this behavior holds true away from the drip-lines, as the Bethe-Weizsäecker has no threshold features on the drip-lines. Therefore the only plausible explanation can be coincidental-agreement.

The Bethe-Weizsäecker formula is good in the "blue lagoon" region, then degrades fast towards the drip-line. The (pseudo)-physics fundament of the Bethe-Weizsäecker formula further diverges from experimental data as the nuclide approaches the drip-line. Still, the Bethe-Weizsäecker formula improves in the same direction of change as the binding energy, giving the observed apparent agreement.

It is evident that towards the drip-line a number of collective effects (cluster-dynamics in particular) take place, raising the ground state close to the continuum and inducing evaporation, fission, gamma radiative transitions, etc.

1.2 Neuromorphic software improvement

This represents a first attempt to model nuclear binding energies with a deep learning neural network on the AME2016 data (3433 nuclei), although efforts on smaller data sets [8] seem to have appeared in parallel with this work.

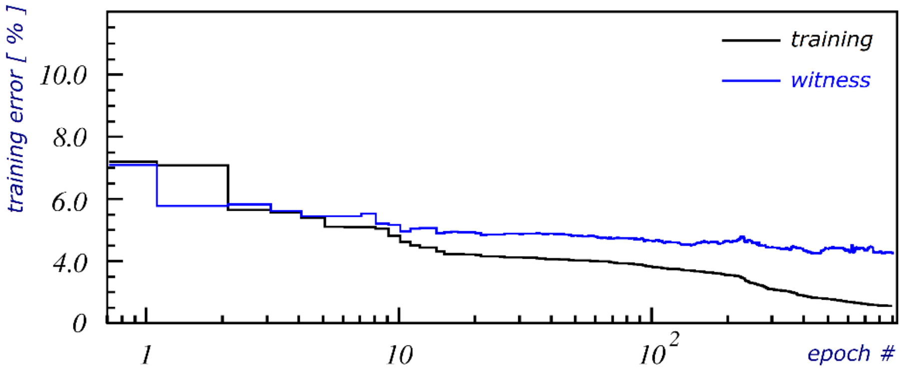

Figure 2: Errors in the training of the Multi-Layer Perceptron network. Training sample in black and test-set sample in blue. Not the relatively prompt departure of the two samples, around 5-8 epochs. The very low training error and its continual vanishing indicate the morphing potential of the MLP, albeit at the cost of losing generality.

I used the MLP neurosoftware package within ROOT [9]. I selected data randomly in two halves and used one for training (using BFGS), while the other as test-set. Figure 2 shows the training errors for the two samples. The overtraining threshold is used as stop criterion, at 10 epochs.

The input parameters to the network were the Bethe-Weizsäecker building blocks: A, Z, $A^{1/2}$, $A^{1/3}$, Z(Z-1), $(A-2Z)^2$, $e^{-A/30}$, etc – in total 7), in order for the network to easily adjust the formula, and also combine those into hereto unknown features. This is for faster convergence. The MLP has the input layer (7 neurons), hidden layer (4 neurons) and output layer (1 neuron).

Figure 2 is a very indicative plot, showing that the neural network has capability to fuse onto the training set, albeit diverging from the test-set. It means that although the morphing capability exists, the net cannot steer into the right direction.

The evaluation result of the neural network, figure 3, is largely independent on the training-run of the neural network. A sum over the full 3433/2 nuclei in the test-set gives an rms-error of roughly 0.03% (for residuals predicted in the 0.01-7% range).

The higher residuals (1-7%) around the magic-numbers are due to the lack of "knowledge" of quantum mechanics in the neural-network. Although neural approaches function in certain contexts for quantum-mechanical problems [10], there is no universally accepted approach.

One alternative is to divide the target space into regions, as mentioned, the network has the ability to fuse to the data, and use a set of networks, each specialised for a particular region. This implies abdicating completely from any desire for a unitary underlying "physics" (even if one "known" only to the neural network).

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The other alternative, as mentioned, is to have sensory parameters, that is formulae with underlying quantum mechanical fundament. They could better sense shell closure and effects on the surface of a closed shell (extra nucleons, or ghost nucleons).

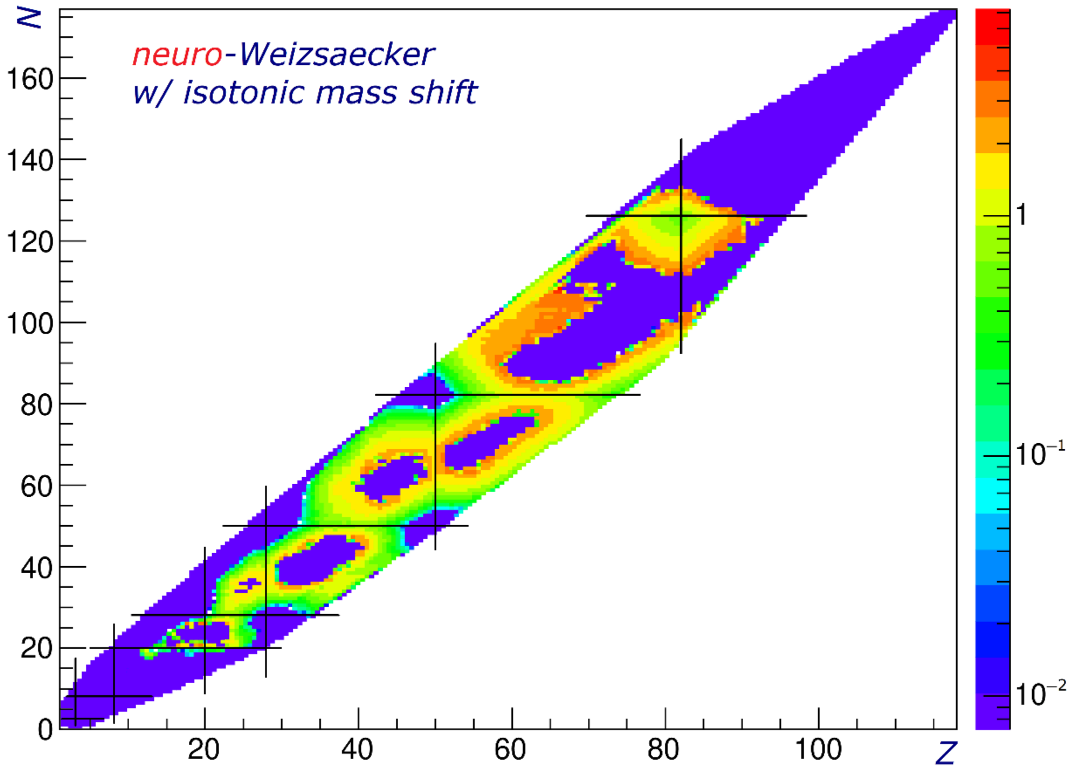

Figure 3: Residuals between experimental data and the neuro-Bethe-Weizsaecker liquid drop formula with isotonic shifts. Colors are %'s.

These aspects are raised by the result plot in figure 3. The neuro-code eliminated all errors in the low mass region, probably by accident, as this clearing of the low-masses region had no impact on the other regions. It also alleviated the red regions, of high errors by some amount.

There is no evidence of the neurocode having discovered any underlying physics correlation across the board.

This is to be expected since quantum mechanical considerations are very non-linear, abrupt and require way more than a few neurons.

References

[1] I. Tanihata, *Neutron halo nuclei*, J. Phys. **G22**, 157 (1996).

[2] K. Heyde, *Basic Ideas and Concepts in Nuclear Physics*, IOP, Bristol, 1999.

[3] I.I. Gurevich, M.I. Pevsner, *Repulsion of nuclear levels*, *Nuclear Physics* **2**, p. 575-581 (1956).

[4] V.V. Sokolov, V.G. Zelevinsky, *On a statistical theory of overlapping resonances*, Phys. Lett. **B202**, p. 10-14, (1988).

[5] D.I. Bonbright et al, *The four-body reaction ^{6}Li(p,pα)np as a probe of the cluster structure of ^{6}Li*, *J. Phys.* **G3**, p. 1359 (1977); Y.T. Oganessian, V.I. Zagrebaev, *Dynamics of two-neutron transfer reactions with the Borromean nucleus* ^{6}He, Phys. Rev. **C60**, p. 044605 (1999).

[6] C. Samanta and S. Adhikari, *Extension of the Bethe-Weizsäcker mass formula to light nuclei and some new shell closures*, Phys. Rev. **C65**, p. 037301 (2002); S. Adhikari and C. Samanta, *Systematic study of shell effect near drip-lines*, IJMPE **13**, p. 987 (2004).

[7] M. Wang, G. Audi, F.G. Kondev, W.J. Huang, S. Naimi, X. Xu, *The AME2016 atomic mass evaluation*, Chinese Phys. **C41**, p. 030003 (2017).

[8] A. Bobyk, W.A. Kaminski, *Deep Neural Networks and the Phenomenology of Super-Heavy Nuclei*, Phys. Part. And Nuclei 53, p. 167-176 (2022).

[9] R. Brun and F. Rademakers, *ROOT - An Object Oriented Data Analysis Framework*, Nucl. Inst. and Meth. in Phys. Res. **A389**, p. 81-86 (1997).

[10] G.A. Nemnes, T.L. Mitran, A. Manolescu, *Gap Prediction in Hybrid Graphene-Hexagonal Boron Nitride Nanoflakes Using Artificial Neural Networks*, J. Nanomat. Vol. 2019, ID 6960787 (2019).

[11] F. Dyson, *A meeting with Enrico Fermi*, F. Dyson, Nature **427**, p. 297 (2004): "*With four parameters I can fit an elephant, and with five I can make him wiggle his trunk*." - attributed to John von Neumann.