Development of a novel EDF for beyond mean-field calculations

Tsukuba-CCS workshop on “microscopic theories of nuclear structure and dynamics”

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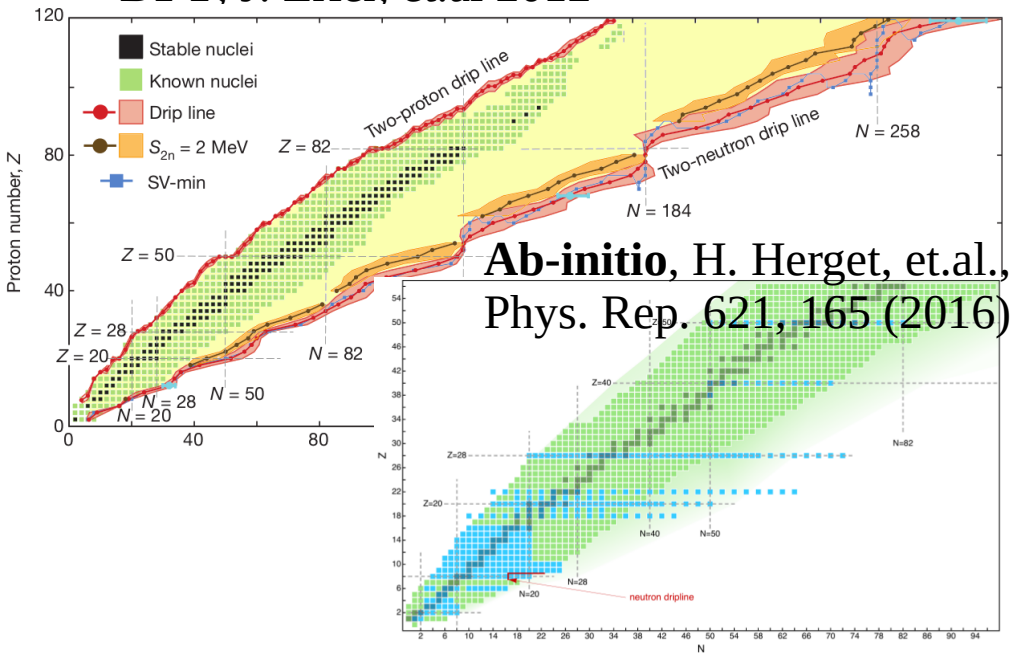
Nuclear DFT and beyond mean-field calculations

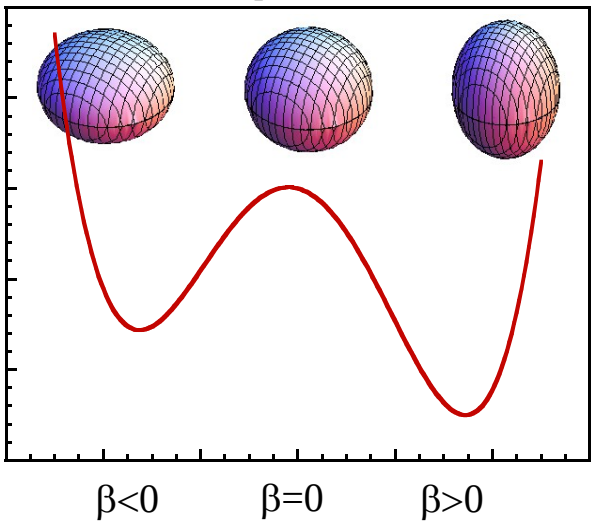
- The nuclear DFT is the only microscopic theory which can be applied throughout the entire nuclear chart
- Important ingredient of nuclear DFT is symmetry breaking (e.g. particle number, rotational symmetry, etc.) which can be used to introduce correlations
- Symmetry broken state is no longer an eigenstate of symmetry operator: It has no good quantum number
- In principle symmetries broken on the mean-field level should be restored with projection

DFT, J. Erler, et.al 2012

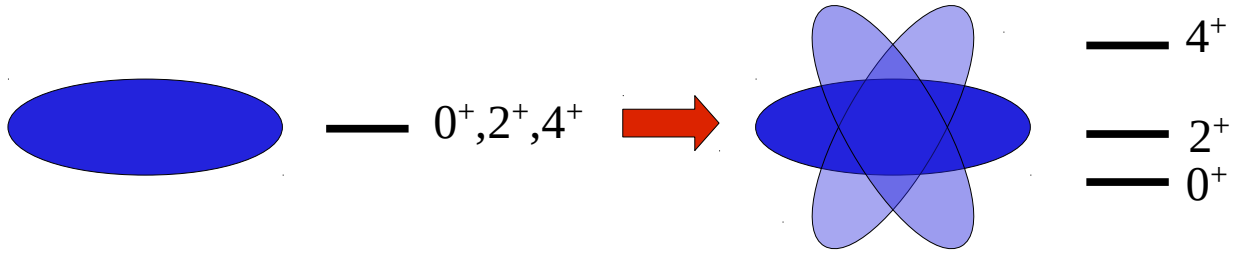


Ab-initio, H. Herget, et.al., Phys. Rep. 621, 165 (2016)

Spontaneous symmetry breaking



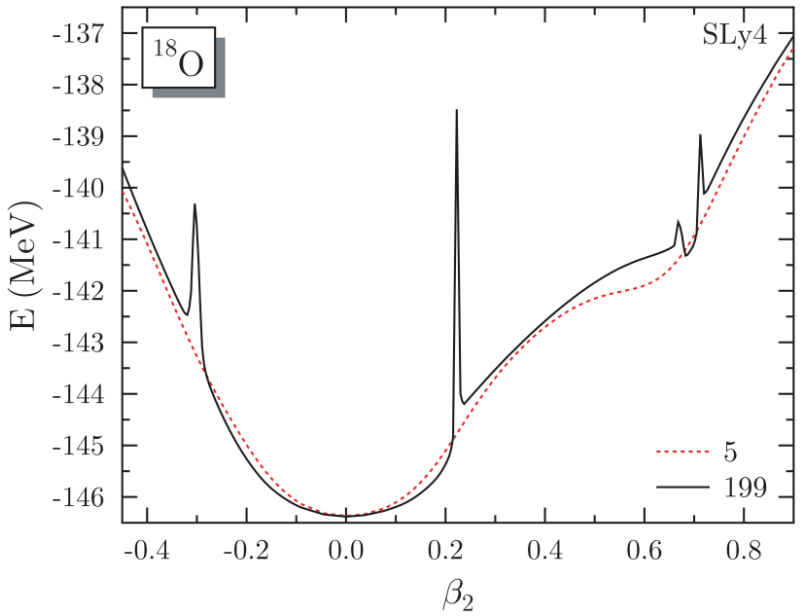
- Schematically, projection includes rotation of the wave-function along the gauge angle(s), weighted with a weight function
- Projection restores symmetry: Projected state has again good quantum number w.r.t. restored symmetry operator



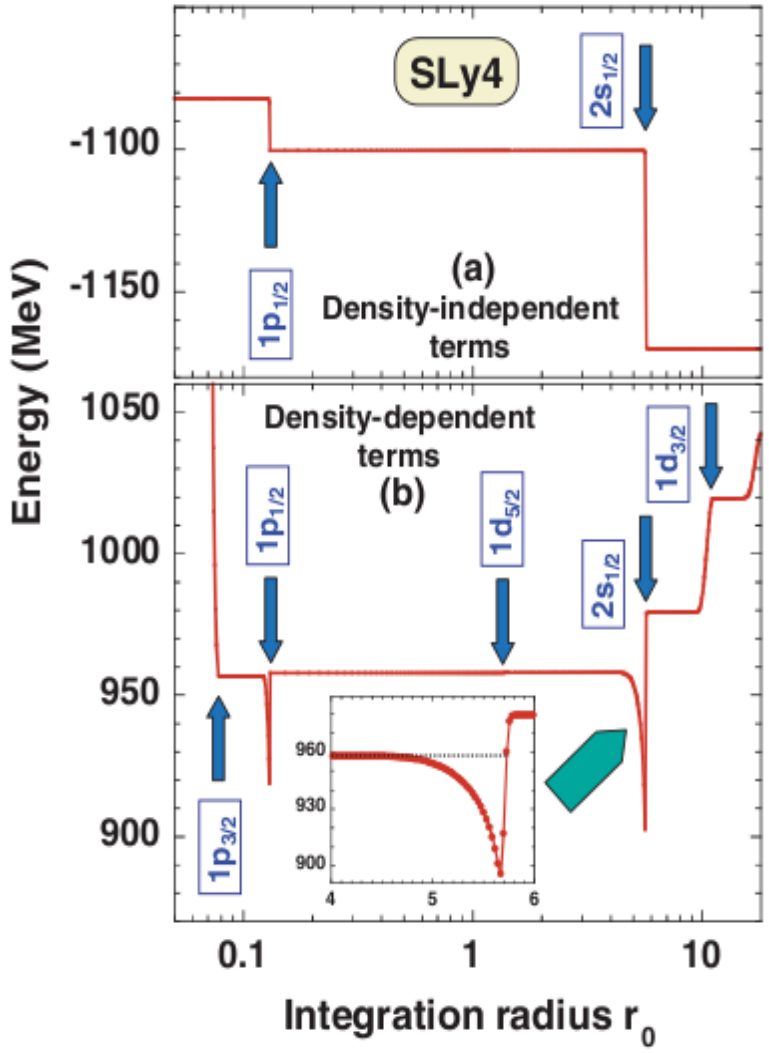
Nuclear DFT and beyond mean-field calculations

- The key ingredient of DFT is the energy density functional (EDF)
- It turns out, that with most of the current EDFs, there are serious problems when trying to project
- Firstly, density dependent term, appearing in most of the EDFs, becomes troublesome with projection. It causes non-analytic behavior of the energy kernels
- Secondly, use of different interaction in ph- and pp-channels leads to self-pairing and other unwanted features

M. Bender, et. al., PRC 79, 044319 (2009)



J. Dobaczewski, et. al., PRC 76 054315 (2007)



- There are some regularization schemes, but they may not work in all cases
- The simplest way to avoid these issues is to use EDF which is strictly based on an underlying effective force!

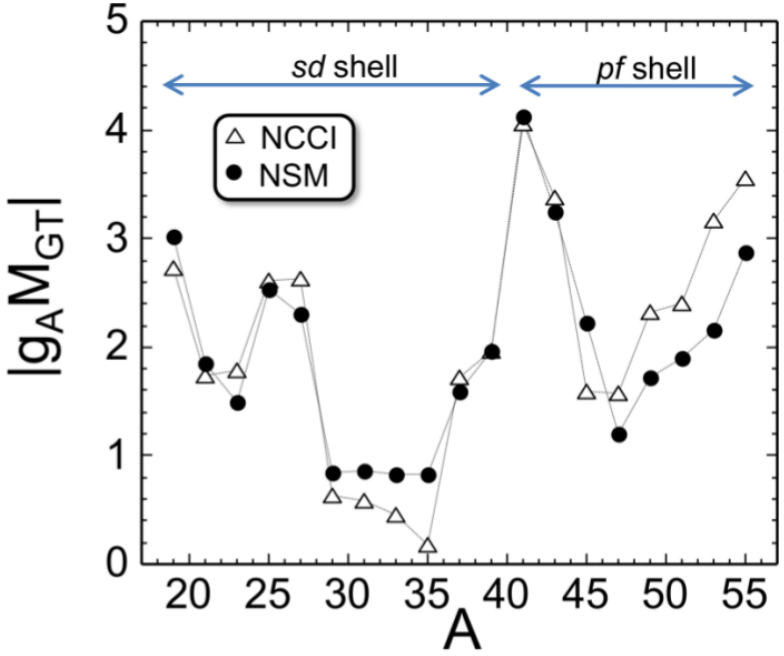
Nuclear EDFs applicable for beyond mean-field calculations

- Old SV force from 1970's, with tensor part included: SV_T. This actually works surprisingly well in beyond mean-field calculations when looking at spectra or beta-decay rates. Weak point: Pairing.

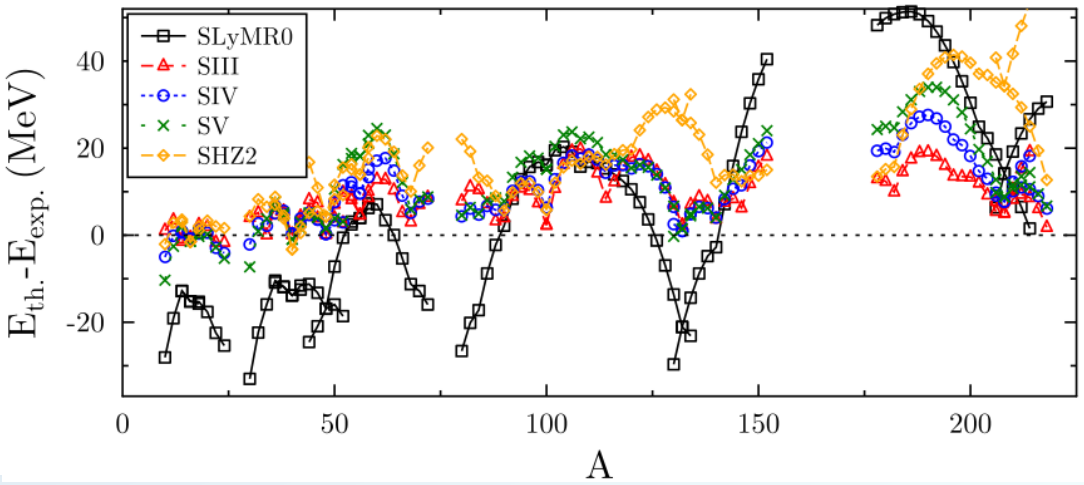
- SLyMR0: Derived from a zero-range 2N, 3N and 4N force. Includes also pp-channel. Weak point: Large arc-like features when looking at binding energy residues

- Finite range pseudopotential based EDF. This is currently been developed. Based on a finite range force and possible contact terms. Possible issue: Calculations computationally more demanding

M. Konieczka, et.al., PRC 93, 042501(R) (2016)
NCCI = DFT-rooted no-core configuration interaction approach. NSM = nuclear shell model



J. Sadoudi, et.al, Phys. Scr. T154 014013 (2013). SLyMR0 residues



Finite range EDF

- First introduced at F. Raimondi, et.al, J. Phys. G 41, 055112 (2014)
- The form of the regularized finite range potential is

$$\mathcal{V}_j^{(n)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \left(W_j^{(n)}\hat{1}_\sigma\hat{1}_\tau + B_j^{(n)}\hat{1}_\tau\hat{P}^\sigma - H_j^{(n)}\hat{1}_\sigma\hat{P}^\tau - M_j^{(n)}\hat{P}^\sigma\hat{P}^\tau\right) \times \hat{O}_j^{(n)}(\mathbf{k}_{12},\mathbf{k}_{34})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})g_a(\mathbf{r}_{12})$$

where $g_a(\boldsymbol{r})$ is a Gaussian with length scale a. Term $\hat{O}^{(n)}$ contains relative momentum operators $\boldsymbol{k}$ of the order n, with n = 0,2,4,6

- For each order of n, the potential contains adjustable parameters $W_j^{(n)}$, $B_j^{(n)}$, $H_j^{(n)}$, and $M_j^{(n)}$.
- In addition to Coulomb and contact spin-orbit term, a zero range two-body term was introduced to obtain better pairing channel properties

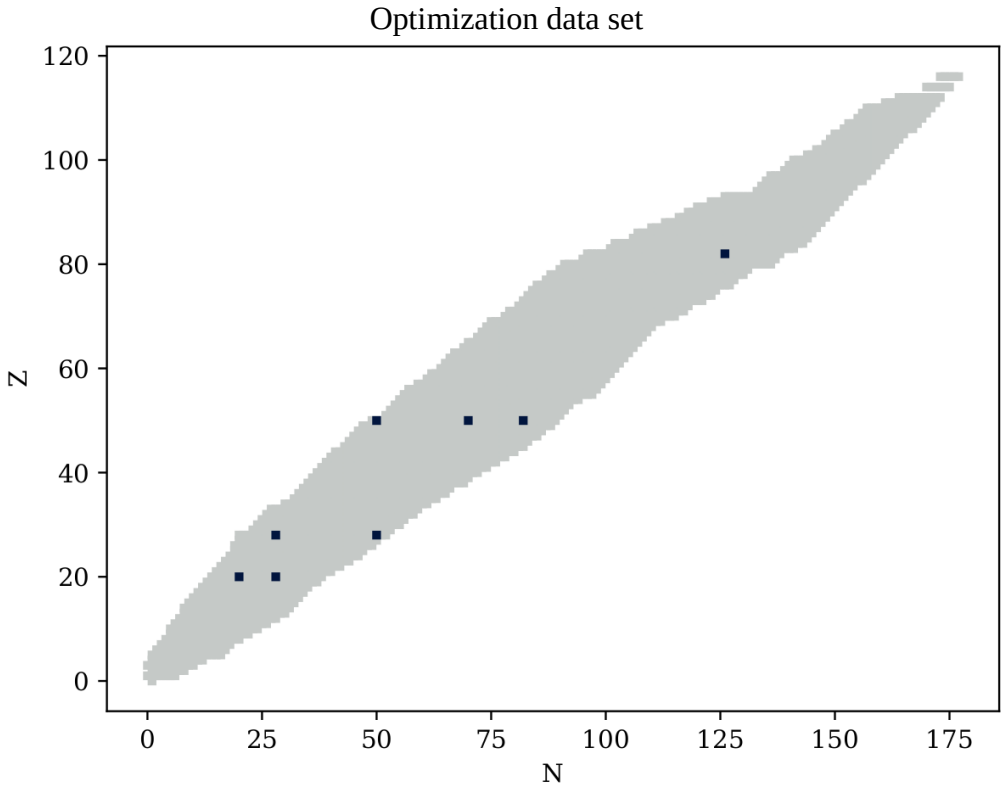
$$\mathcal{V}_\delta(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = t_0\left(1+x_0\hat{P}^\sigma\right)\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})$$

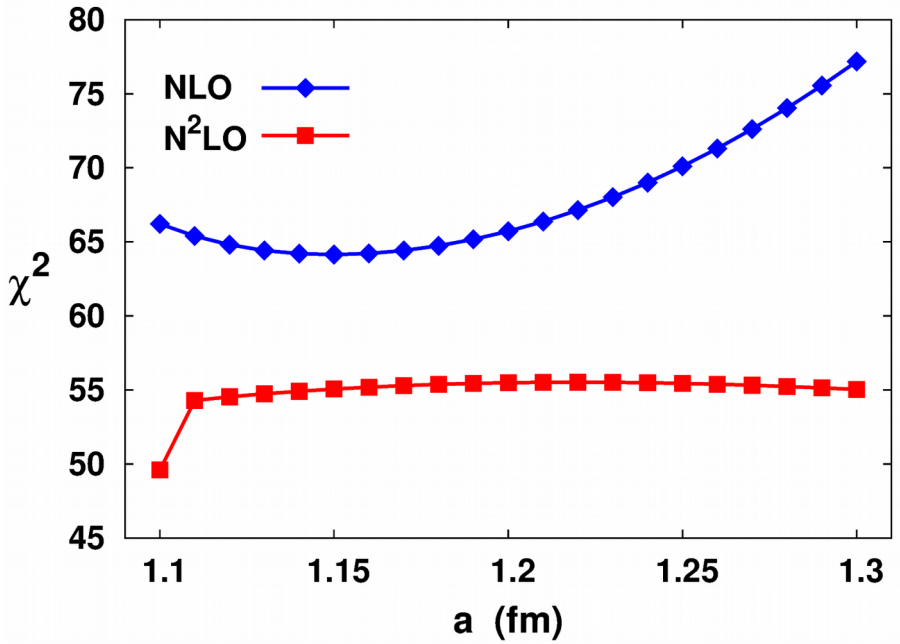
- This potential is used as a generator for the EDF for both, particle-hole and particle-particle channels. The EDF is strictly based on the underlying force

Finite range EDF, first parameter optimization

- First set of optimized parameters published recently: K. Bennaceur, A. Idini, J. Dobaczewski, P. Dobaczewski, M. Kortelainen, and F. Raimondi, J. Phys. G 44, 045106 (2017). Optimization at spherical HFB level with coordinate space based HFB solver

- Optimization data set contained masses of spherical nuclei, radii, pairing gap, and some constraints on infinite nuclear matter. At N2LO level, the χ^2 depends only weakly on the length scale *a*
- Parameter uncertainty analysis was done for obtained parameters

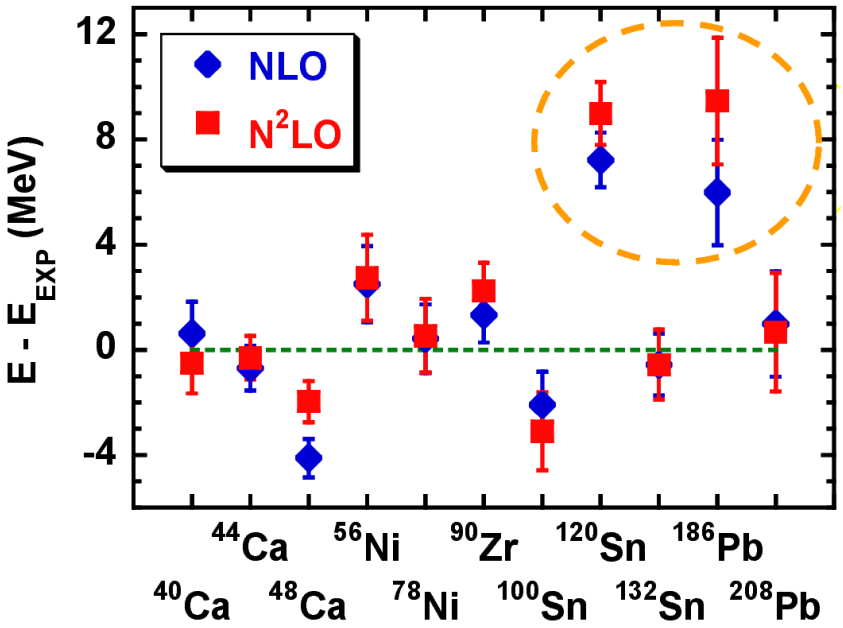




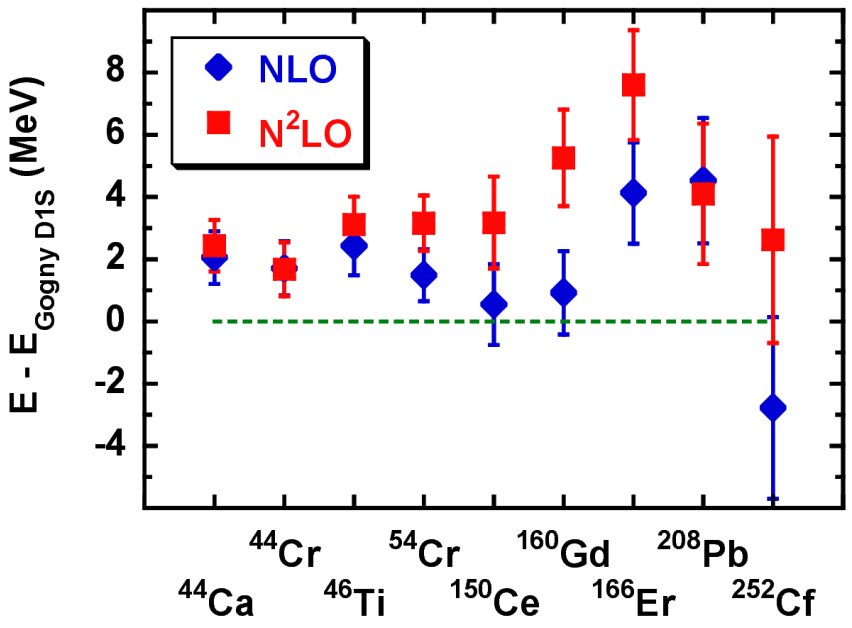
Results from the first optimization

- Binding energy for spherical doubly-magic nuclei is usually rather well reproduced, since these were also in the input data set
- At mid-shell, small effective mass deteriorates predicted binding energies
- For deformed nuclei, propagated uncertainties become larger

Binding energies with propagated errors compared to experimental values



Binding energies with propagated errors compared to Gogny D1S

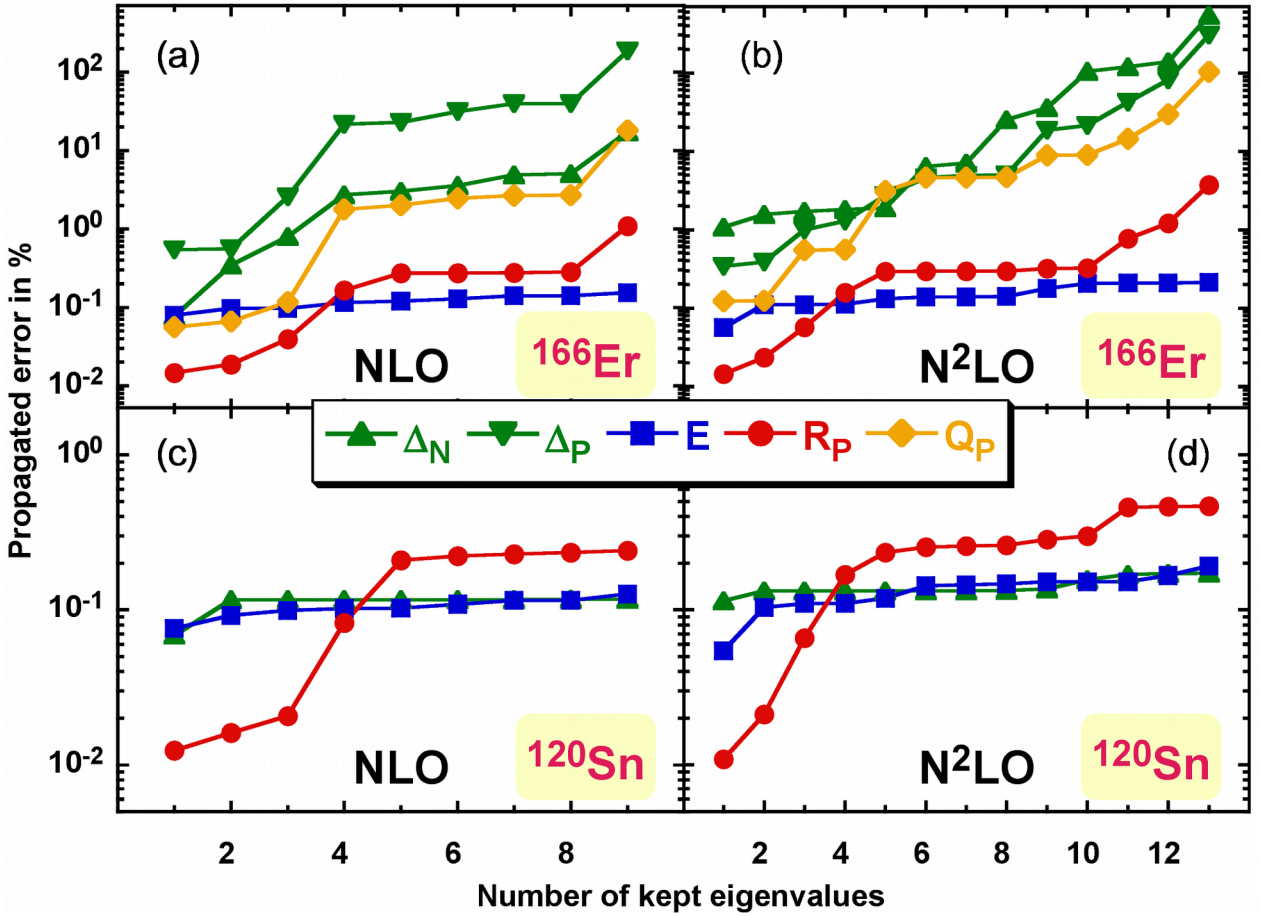


Propagated error and deformed nucleus

- A closer inspection shows that propagated error for some observables in deformed ^{166}Er becomes large
- Current input data can not constrain parameters which are strongly connected to these observables

- To fix these issue with deformed nuclei, the next step is to use data on deformed nuclei
- This optimization is done with newly developed HFB code called HFBtemp, combined with POUNDerS algorithm for parameter optimization at deformed HFB level

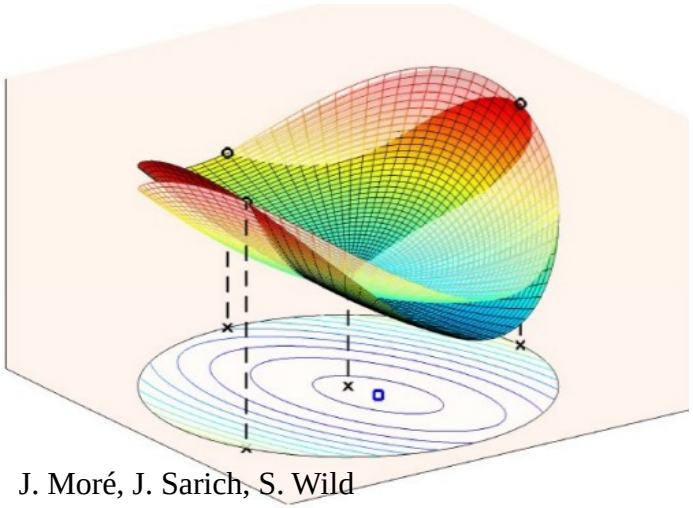
Propagated error as function of number of eigenvalues kept when computing covariance matrix.



Tools of the EDF parameter optimization

POUNDerS

- A quasi-Newton based parameter optimization algorithm
- Builds a local model of each element in the χ^2 function, within a trust region
- Locates minimum significantly faster than Nelder-Mead algorithm
- Has been applied to many problems in nuclear physics and other domains



J. Moré, J. Sarich, S. Wild

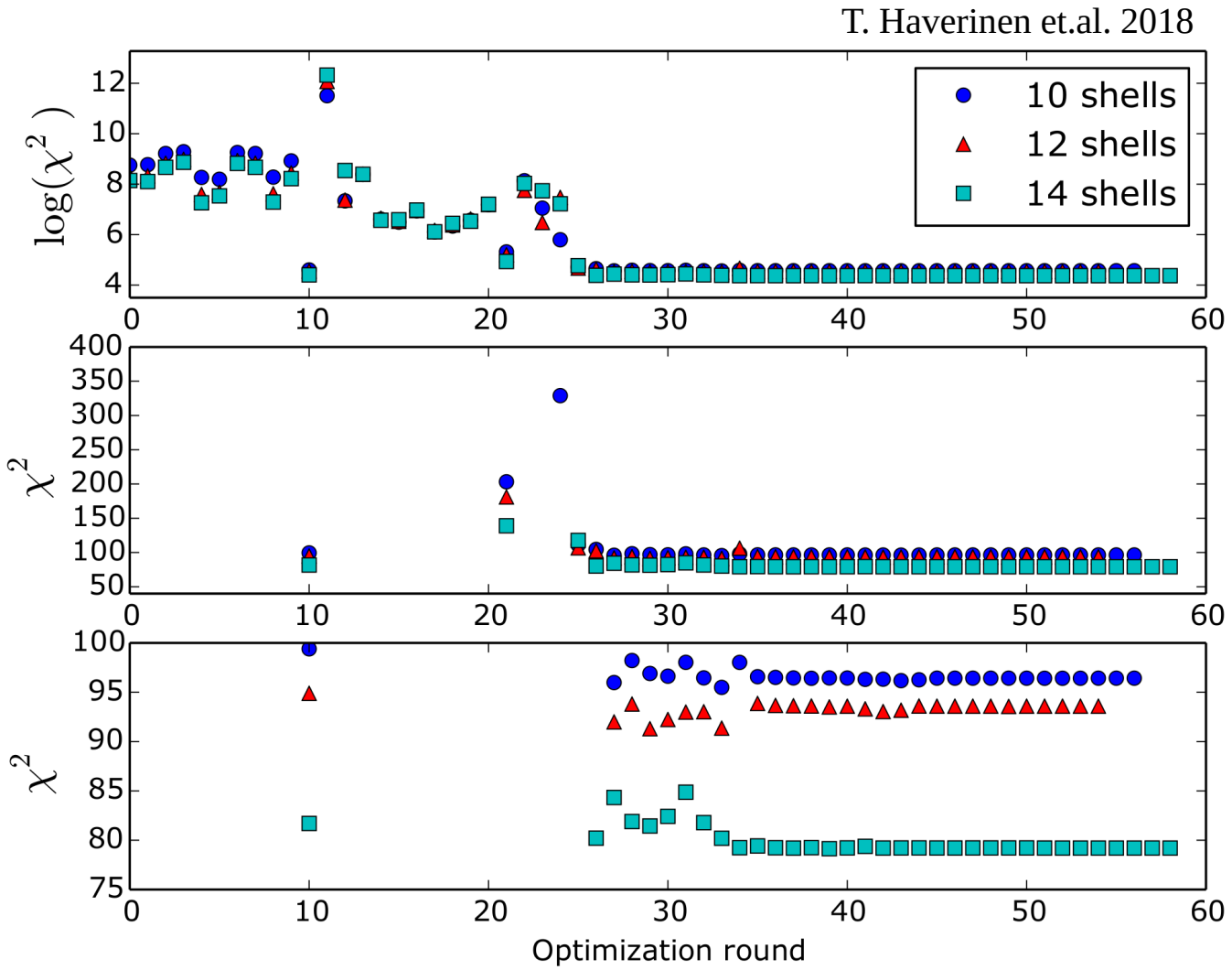
- S. M. Wild, Solving Derivative-Free Nonlinear Least Squares with Pounders, Report No. ANL/MCS-P5120-0414, Argonne National Laboratory

HFBtemp

- Recently developed HFB code
- Goal is to build a modular HFB code, in which one could freely combine various bases (axial, 3D Cartesian, ...) with various EDFs (Skyrme, finite range, ...), and later with other components
- Written in c++, uses a lot of template programming structures.
- Contains presently Skyrme EDF for axial and 3D case and finite range EDF for axial case.
- Successfully benchmarked against HFODD
- Parallelized with OpenMP and MPI

Testing optimization at deformed HFB level

- To test the optimization setup, we used first earlier data set, consisting only spherical nuclei

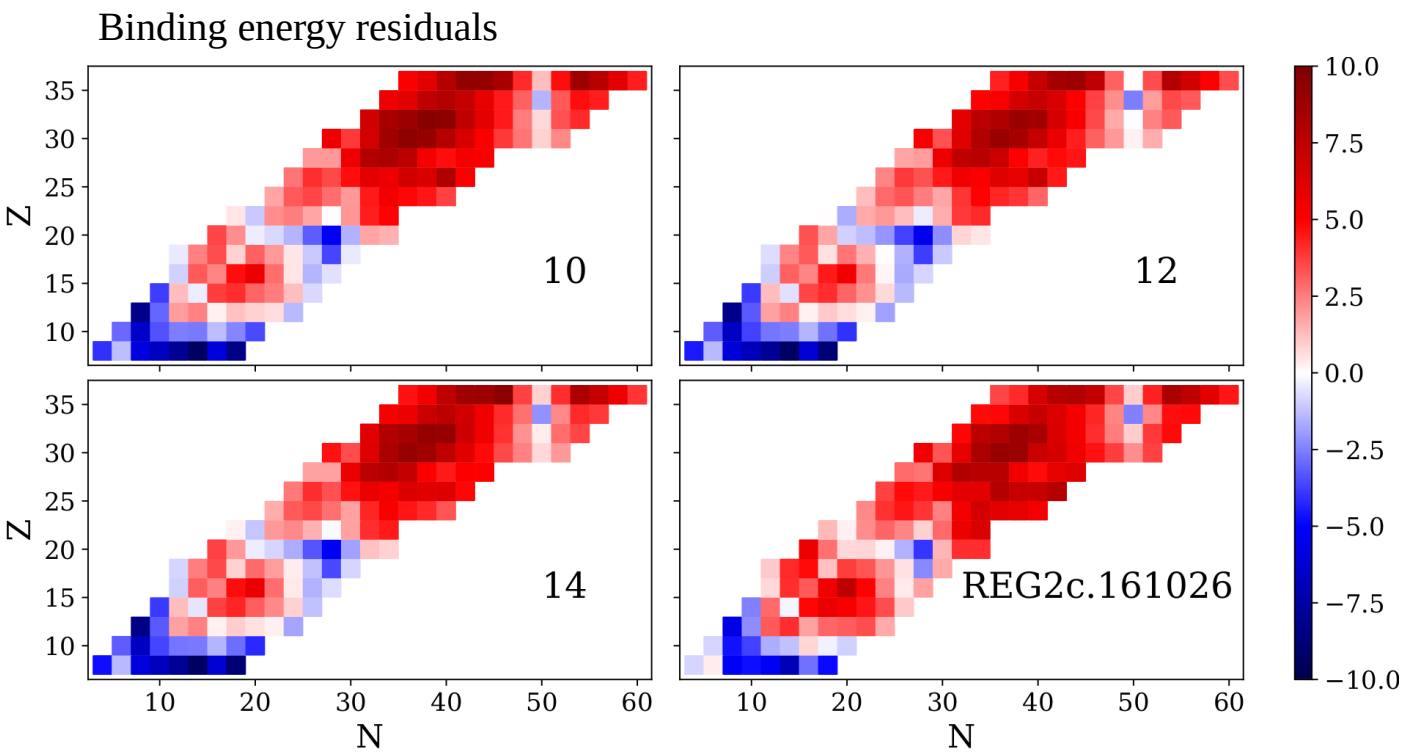


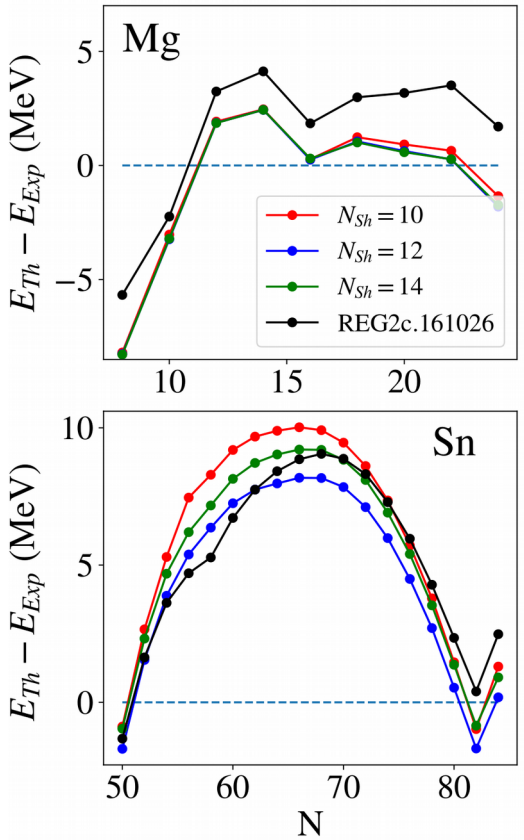
- Test optimization works as intended. Optimization routine converges to minimum rather quickly

Testing optimization at deformed HFB level

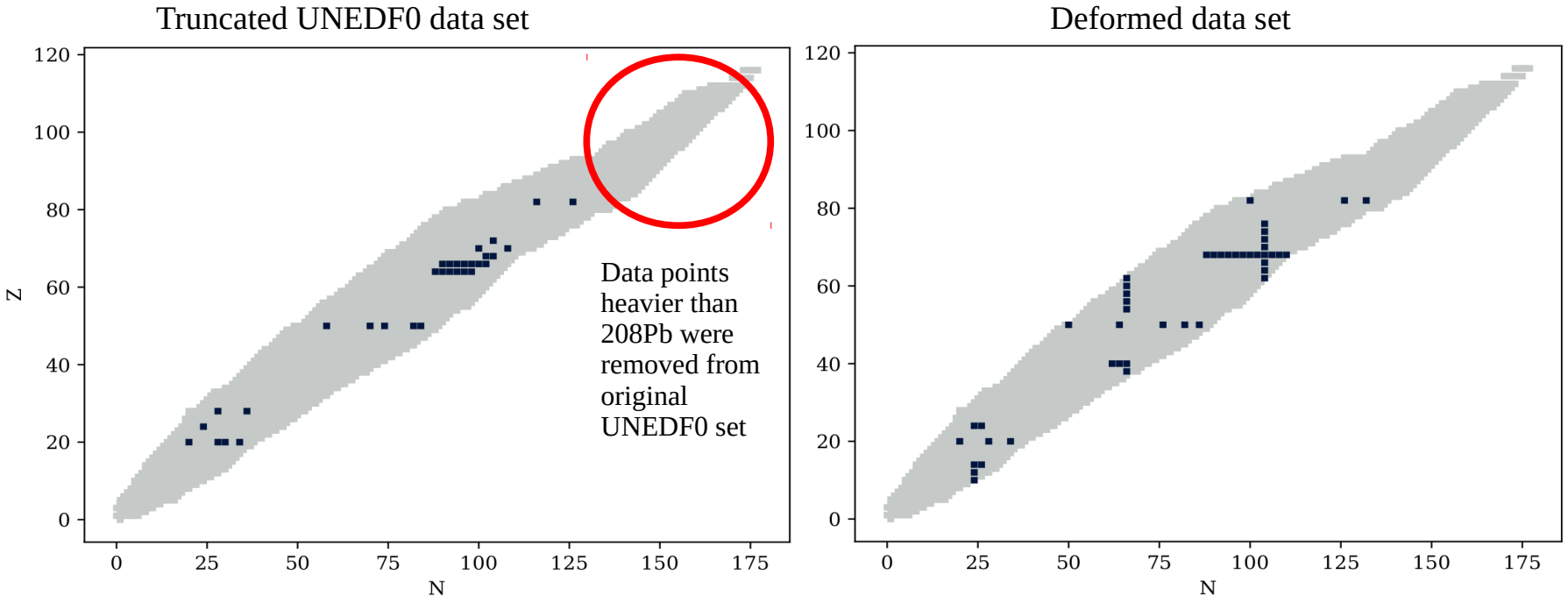
- We tested the impact of used basis size on resulting optimized parameter set
- Parameter values, when using 10, 12, or 14 oscillator shells, differed somewhat from each other
- When calculating predictions with each EDF, by using the same setup as in optimization, the results were very similar
- The effects coming from used basis size can be, in some degree, effectively absorbed in the optimized parameter set

T. Haverinen, M. Kortelainen, J. Dobaczewski, K. Bennaceur, arXiv:1811.02997, 2018





Optimization at deformed HFB level



- Next step: Use data on deformed nuclei
- Two deformed data sets were tested: Truncated UNEDF0 data set and a set containing mid-shell isotopic and isotonic chains of nuclei
- No infinite nuclear matter properties included in χ^2 function
- Optimization failed for both of these sets. EDF parameters drifted to unstable region

⇒ Constrains on infinite nuclear matter properties, or generally, data on nuclear EoS required for successful optimization

Conclusions and future plans

- The goal is to obtain an EDF, based on a finite range pseudopotential, applicable for multi-reference beyond mean-field DFT calculations
- The first set of parameters was optimized at spherical HFB level. Gives rather good description of most spherical nuclei. However, uncertainties with deformed nuclei were larger
- The second optimization round at deformed HFB level encountered problems. Seems to require input from nuclear EoS

Future plans

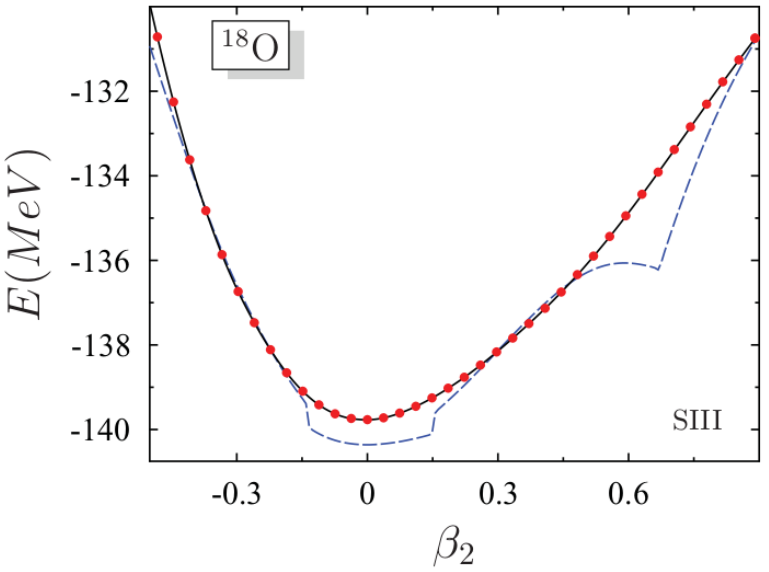
- Readjust deformed optimization scheme
- Address the problem of low effective mass
- Large scale mass table survey

Backup slides

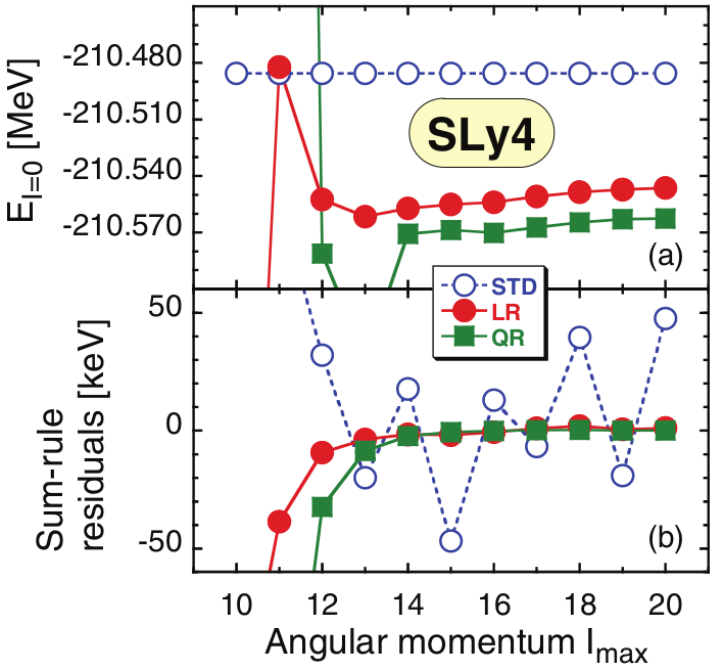
EDF regularization procedures

- Various regularization techniques have been developed for particle number and angular momentum projections. These methods remove singular behavior
- So far, it is unclear if these techniques can be combined to simultaneous restoration of both symmetries in all possible cases
- Use of Gaussian overlap approximation also regulates kernel. However, no formulation exists for odd-odd collective Hamiltonian model
- Therefore, to solve these issues, the most simplest solution is to generate an EDF which is strictly equivalent to underlying force. This prevents singularities during projection.
- Both ph-, and pp-part of the EDF should come from the same underlying force.

G. Hupin, et. al., PRC 84, 014309 (2011)



W. Satuła, J. Dobaczewski, PRC 90, 054303 (2014)



Parameterization

Table 3. The NLO and N^{2}LO coupling constants of local pseudopotentials (3) and (7) regularized at $a = 1.15\,\mathrm{fm}$. (in MeV fm^{n+3}) shown together with their statistical errors.

Order	Coupling Constant	NLO REG2c.161026	N^{2}LO REG4c.161026
$n=0$	$W_1^{(0)}$	41.678375±0.6	3121.637124±1.5
	$B_1^{(0)}$	−1405.790048±4.3	−4884.029523±1.8
	$H_1^{(0)}$	202.879894±4.1	3688.310059±2.9
	$M_1^{(0)}$	−2460.684507±6.7	−5661.028710±2.8
$n=2$	$W_1^{(2)}$	−79.747992±4.2	547.802973±1.9
	$B_1^{(2)}$	73.112729±1.4	−319.513120±1.3
	$H_1^{(2)}$	−681.295790±3.2	−134.164127±0.3
	$M_1^{(2)}$	−48.161707±5.1	−318.407541±0.6
$n=4$	$W_1^{(4)}$		2019.945667±2.2
	$B_1^{(4)}$		−2365.956384±1.6
	$H_1^{(4)}$		2310.445509±1.8
	$M_1^{(4)}$		−2117.509518±4.0
	W_{SO}	177.076480±4.7	174.786236±5.1

In addition a contact term

$$\mathcal{V}_\delta(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = t_0\left(1+x_0\hat{P}^\sigma\right)\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{24})\delta(\mathbf{r}_{12})$$

with $x_0 = 1$, $t_0 = 1000$ MeV fm^3.