EDFs for beyond mean-field calculations

Uncertainty quantification in nuclear physics
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MITP, Mainz

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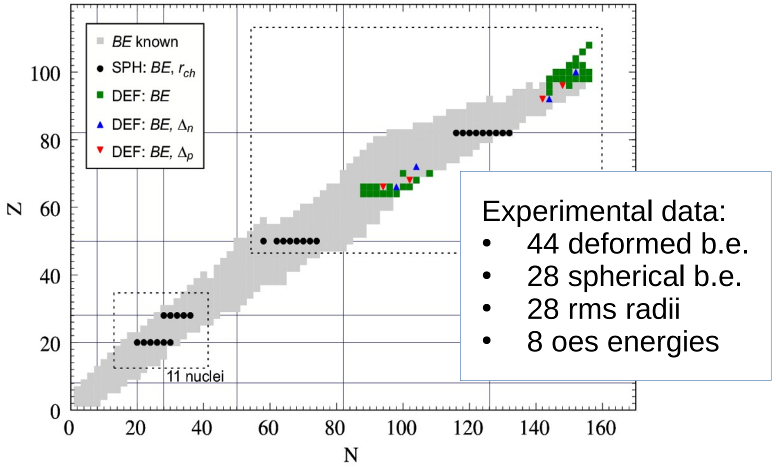
Spoiler: We don’t have yet an EDF which would work well enough in all such kind of calculations

But we have an idea how to construct one and are working towards it

DFT based models

- DFT is one of the most flexible many-body approach
- Key element in DFT is the energy density functional (EDF). It encodes complex nuclear interactions into energy density
- Parameters of the EDF needs to be adjusted to empirical input. Some parameters better constrained than others. For example, time-odd part of the EDF not so well constrained

UNEDF0 dataset. M.K. et al, PRC 82, 024313 (2010)



- To solve the many-body wave function, one needs to solve Hartree-Fock-Bogoliubov (HFB) equations. This gives quasiparticle states, the self-consistent mean-field $h = t + \Gamma$, and pairing field Δ.

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_n \\ V_n \end{pmatrix} = \mathrm{E}_n \begin{pmatrix} U_n \\ V_n \end{pmatrix}$$

- The fields are obtained from density matrix ρ and pairing tensor κ, which then are constructed from HFB amplitudes *U* and *V*. The *U* and *V* define the generalized Bogoliubov transformation

$$\Gamma_{ab} = \sum_{cd} \bar{v}_{adbc} \rho_{cd}$$

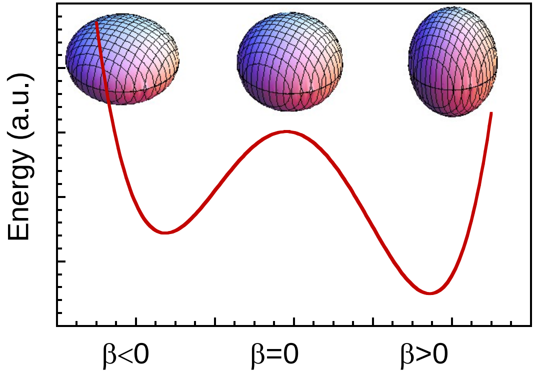
$$\Delta_{ab} = \frac{1}{2} \sum_{cd} \bar{v}_{abcd} \kappa_{cd}$$

$$\rho = V^* V^T , \quad \kappa = V^* U^T$$

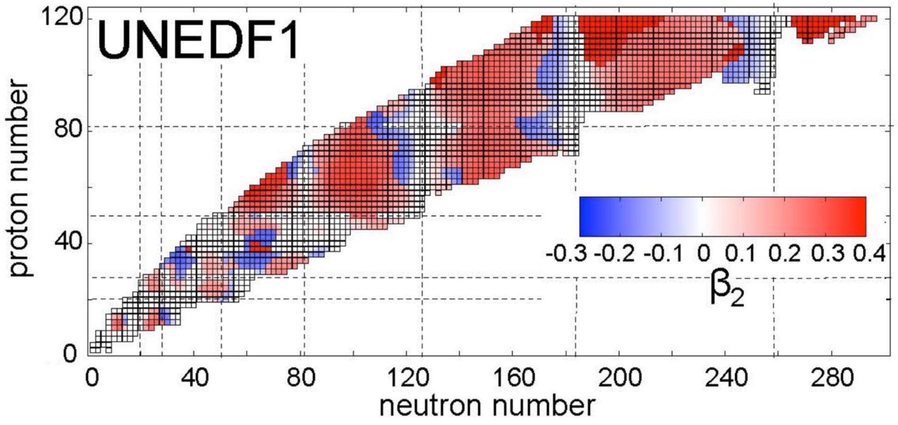
- HFB equations can be solved by using a set of basis states or in coordinate space. These are nonlinear equations and needs to be solved iteratively

DFT based models, spontaneous symmetry breaking

- Spontaneous symmetry breaking is important element in the DFT.
- Allows to effectively incorporate various correlations into the wave-function. Examples: nuclear deformation (rotational symmetry) or nuclear superfluidity via pairing in HFB (U(1) symmetry)
- It turns out that most of the nuclei are deformed and most of the nuclei are in superfluid state



Quadrupole deformation. J Erler et al, Nature 486, 509 (2012).



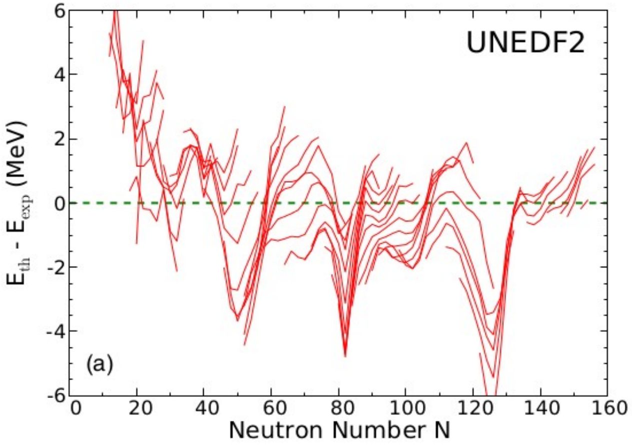
- In principle, symmetries broken at mean-field level should be restored. This is computationally costly and has been often neglected.
- Symmetry broken state is not an eigenstate of corresponding symmetry operator. Therefore, it is not meaningful to compute certain observables (e.g. broken rotational symmetry and magnetic moment)
- Symmetry broken mean-field state is referred as a single-reference (SR) state

Skyrme EDF and its limits

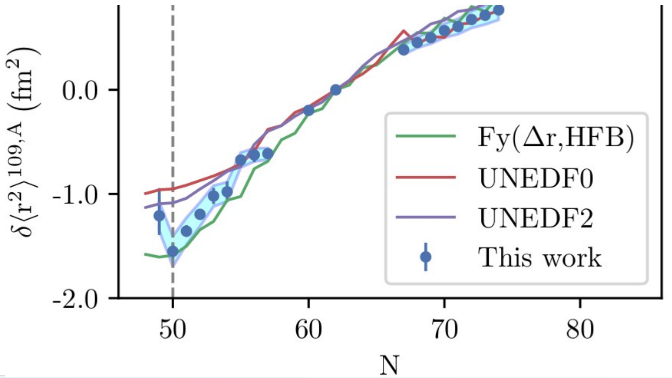
- Skyrme EDF is obtained from a zero-range Skyrme force. Supplemented with Coulomb and pairing EDF
- Has density dependent part. Mean field part and pairing part usually from different effective interaction
- Has been applied to many phenomena (nuclear bulk properties, fission, collective models, linear response, …)

- With various nuclear bulk properties, SR Skyrme EDF approach can usually reproduce general trend, but may have difficulties with local variation
- Spectroscopic quality of SR Skyrme EDF approach can not be improved any further
- Can have serious problems in beyond mean-field calculations (although some cases seems to be ok)

UNEDF2 binding energy residuals.
M.K., et al, PRC 89 054314 (2014)



Isotopic shifts of chr. radius in Ag, M. Reponen, et al, Nature Comm 12, 4596 (2021)



Why do we want to go beyond mean-field?

- Improve predictions for various nuclear bulk properties
  - Better reproduction of local variation of various observables (hopefully...)
  - Better input for various astrophysical simulations (r-process, ...)

- Good quantum numbers
  - Mandatory, for example, for nuclear EM moments and transitions

- Shape coexistence and configuration mixing
  - By definition, multiple mean-field states required
  - Required to explain properties of certain low-lying states (see e.g. various collective models)

- Transition rates and spectroscopy
  - Linear response (QRPA) or cranking can access only certain set of states
  - A lot of exp. data available to test EDF models

Symmetry restoration

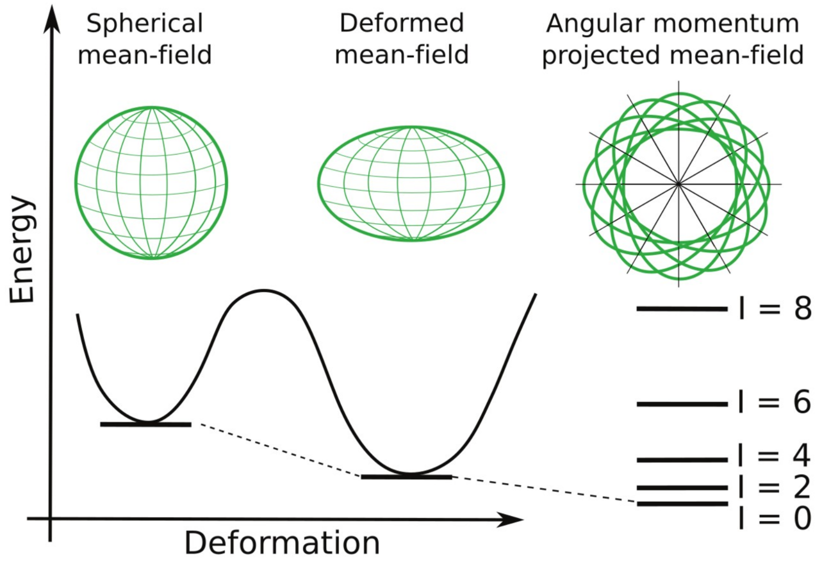
- A symmetry restored wave-function $|\Psi\rangle$ can be constructed from symmetry broken state $|\Phi\rangle$ via projection techniques
- This is done by integrating up over all gauge angles Ω the rotated SR wave-function with a proper weight function $D(\Omega)$. The weight function depends on the restored symmetry, and on which quantum number the restoration is done.

- Since this state is now a linear combination of multiple single-reference states, it is called as a multireference (MR) state

- The energy of this MR wave-function typically depends on the quantum number which is obtained in this process
- For example, restoration of angular momentum for different values of J usually results typical rotational band-like energies.

$$|\Psi\rangle = \int d\Omega D(\Omega)\hat{R}(\Omega)|\Phi\rangle = \hat{P}|\Phi\rangle$$

$$E = \frac{\langle\Phi|\hat{H}\hat{P}|\Phi\rangle}{\langle\Phi|\hat{P}|\Phi\rangle} = \frac{\int d\Omega D^*(\Omega)H(\Omega)}{\int d\Omega D^*(\Omega)N(\Omega)}$$



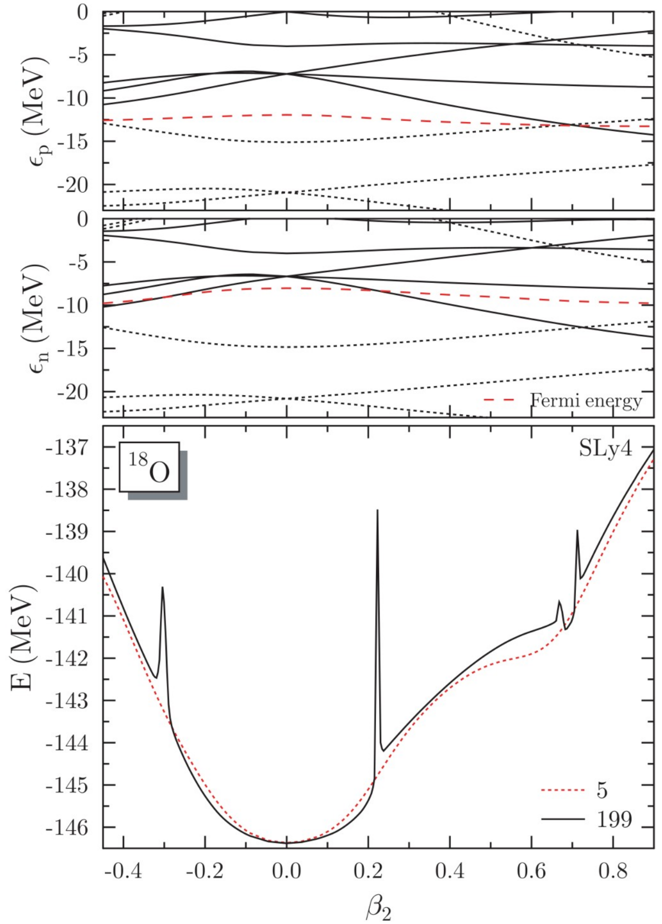
Deformation and angular momentum restoration schematically. From Energy Density Functional Methods for Atomic Nuclei

Singularities in the energy kernel

- When used EDF is not strictly equivalent to underlying force, singularities may appear on kernels with certain values of gauge angle
- This is the case, for example, with density dependent terms or use of different interaction in particle-hole and particle-particle channels
- This leads, for example, to a discontinuous energy surface when some collective parameter is varied.

- This problem does not appear for one-body operators. Total energy, however, is computed at least from two-body operator

- There are techniques to regularize the energy kernel, but it is not certain they will work in all possible cases
- Gaussian overlap approximation regularizes kernels, but collective Hamiltonian models are usually limited to certain kind of cases (like even-even nuclei)



Particle number projected deformation energy with 5 and 199 gauge points. M. Bender et al, Phys Rev C 79, 044319 (2009)

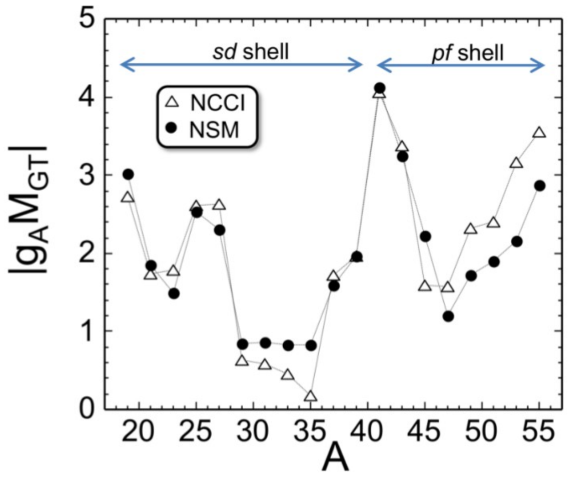
Nuclear EDFs applicable for beyond mean-field caluclations

- 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 on light – medium-light nuclei
  Weak point: Pairing, symmetry energy, effective mass

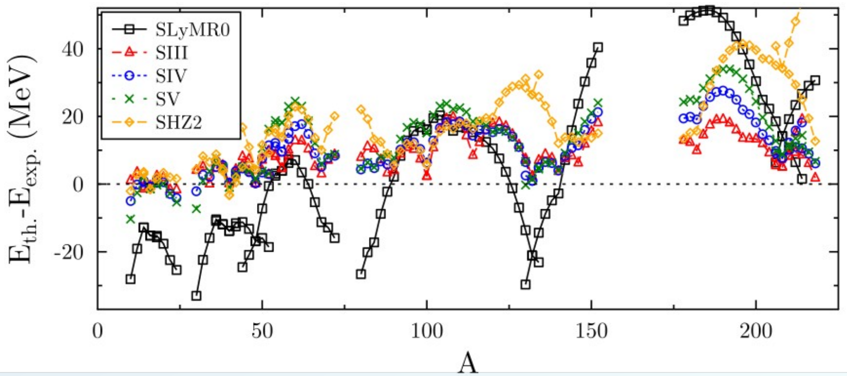
- SLyMR0 and SLyMR1: Derived from a zero-range 2N, 3N and 4N force. Includes also pairing-channel.
  Weak point: Large arc-like features when looking at binding energy residues

- Finite range pseudopotential based EDF. This is currently been developed.

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



What is required from an EDF designed for MR calculations?

- No singularities in the energy kernel in MR calculation
  ⇒ The EDF should be strictly equivalent to an underlying effective force
  ⇒ Same interaction in the particle-hole and particle-particle channel

- Zero-range interactions requires pairing regularization. This is often done with use of pairing window, which violates unitarity of the generalized Bogolibov transformation
  ⇒ Regularization via two-basis method
  or
  ⇒ Use finite range effective force

- Reasonable infinite nuclear matter properties and effective mass
  ⇒ Effective three-nucleon force required

- Reasonable pairing properties
  ⇒ Use finite range effective force, also for 3N part
  (use of zero-range 3N force seems to lead very strong non-local component of κ)

- Good reproduction of nuclear bulk properties, EM moments, and spectroscopy
  ⇒ Parameter adjustment strategy

Finite range pseudopotential based EDF

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

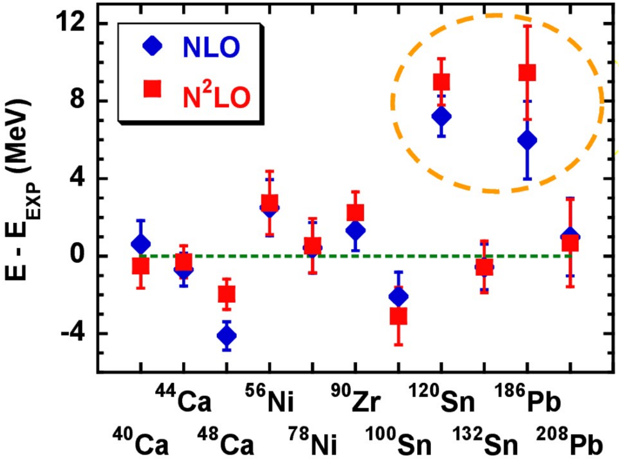
$$\mathcal{V}_j^{(n)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = \left(W_j^{(n)} \hat{1}_\sigma \hat{1}_\tau + B_j^{(n)} \hat{1}_\tau \hat{P}^\sigma - H_j^{(n)} \hat{1}_\sigma \hat{P}^\tau - M_j^{(n)} \hat{P}^\sigma \hat{P}^\tau \right) \times \hat{O}_j^{(n)}(\mathbf{k}_{12}, \mathbf{k}_{34})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

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

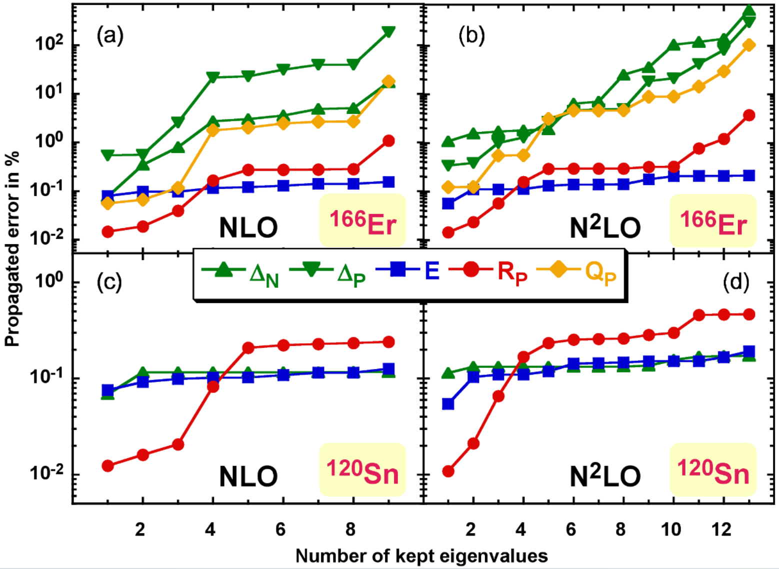
- For each order of n, the potential contains adjustable parameters $W_j^{(n)}$, $B_j^{(n)}$, $H_j^{(n)}$, and $M_j^{(n)}$.
- Compared to zero-range Skyrme force, δ-function has been changed to a finite range Gaussian, which allows now four spin-isospin channels
- This potential is used as a generator for the EDF for both, particle-hole and particle-particle channels
- In addition, Coulomb and spin-orbit required.

Finite range pseudopotential based EDF, first adjustment

- Parameter optimization with data set of 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*
- 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



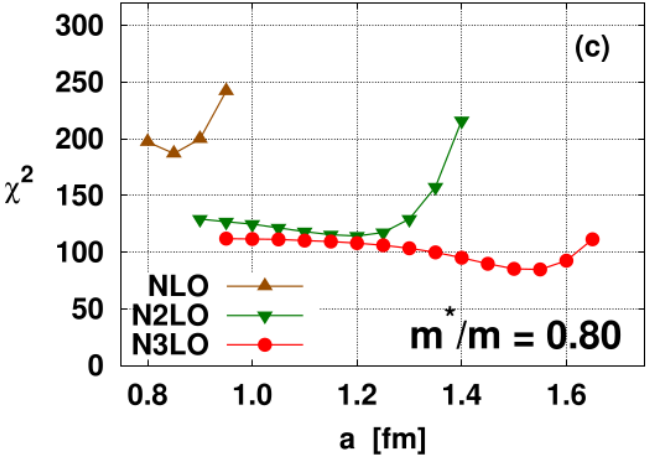
- A closer inspection shows that propagated error for some observables in deformed ^{166}Er becomes large
- Used input data could not constrain parameters which are strongly connected to these observables



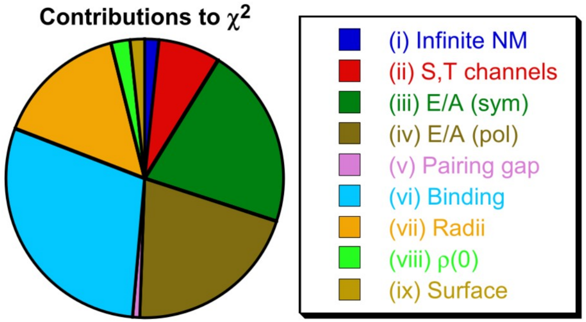
K. Bennaceur, A. Idini, J. Dobaczewski, P. Dobaczewski, M.K., F. Raimondi, J. Phys. G 44, 045106 (2017).

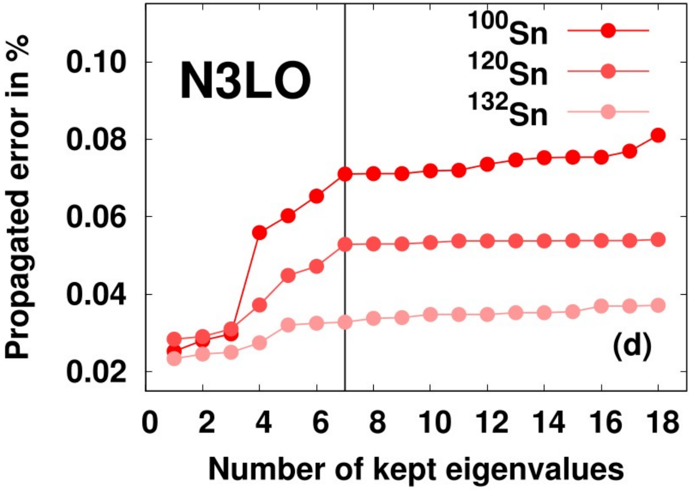
Finite range pseudopotential based EDF, second adjustment

- More robust data set: Infinite nuclear matter properties, spherical nuclei, central densities in ^{208}Pb and ^{40}Ca, and surface energy coefficient
- Adjusted for multiple different eff. mass value *m*/m*
- The final χ^2 value depends very weakly on regularization length scale *a* when going to higher order
- The error budget for final χ^2 value consist mostly nuclear binding energies and various properties of infinite nuclear matter



- When looking propagated errors for binding energies, most of the error is accumulated from 6 – 7 parameter combinations (from NLO to N3LO)

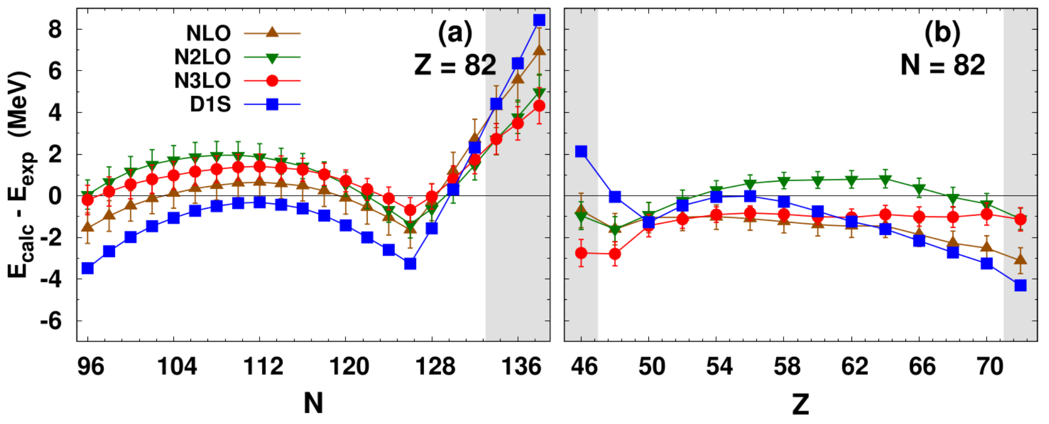


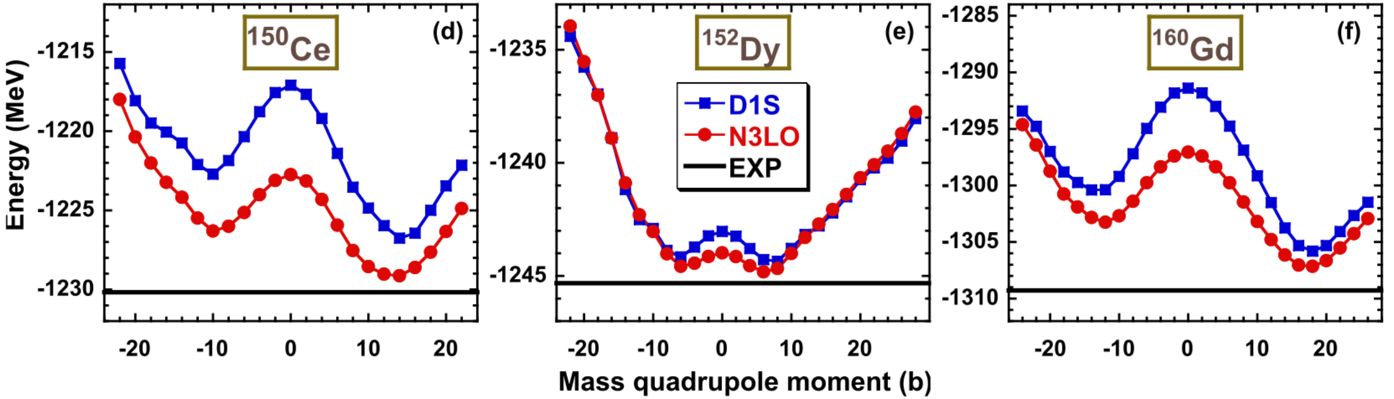


K. Bennaceur, J. Dobaczewski, T. Haverinen, M.K., J. Phys. G 47, 105101 (2020).

Finite range pseudopotential based EDF, second adjustment

- The adjusted N3LO EDF can describe various nuclear properties similarly or better than the standard Gogny or Skyrme functionals.
- Arc-like features present in binding energy residuals. Propagated uncertainties do not always overlap exp. values
- Deformation properties similar to Gogny D1S EDF
- Resulting single-particle spectra depends on eff. mass m^*/m
- Includes density dependent term, which should be removed in next phase





K. Bennaceur, J. Dobaczewski, T. Haverinen, M.K., J. Phys. G 47, 105101 (2020).

Finite range pseudopotential based EDF, 3-body force

- Earlier EDF optimization included density dependent term. This can lead to singularities in any beyond mean-field calculation involving two-body operators (binding energy, configuration mixing, etc.)

- To fix the issue, we are currently developing a semi-contact three-body force based EDF. The generator has form

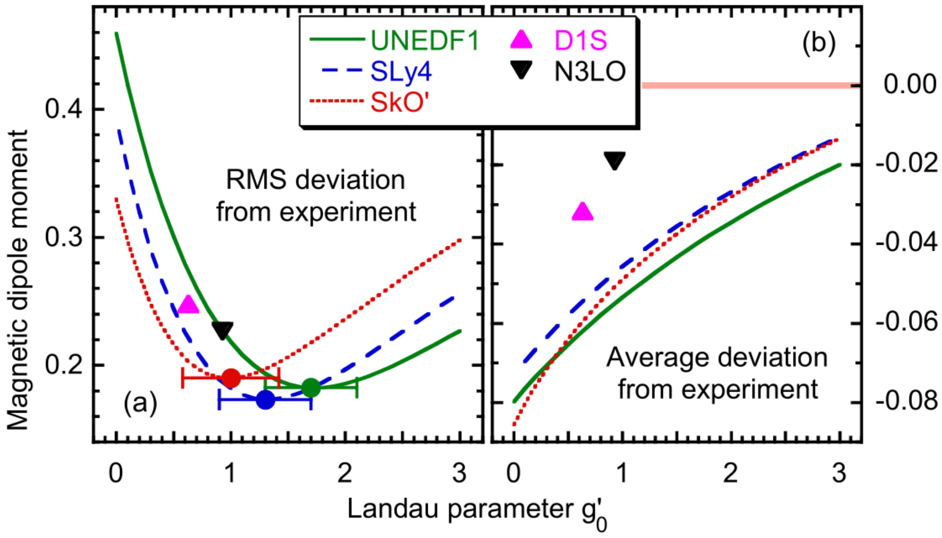
$$\mathcal{V}^{3N} = \frac{1}{6} W^{3N} \left(g_\alpha(|\mathbf{r}_1 - \mathbf{r}_2|)\delta(\mathbf{r}_2 - \mathbf{r}_3)(1 + xP_{\sigma_2,\sigma_3}) + \text{permutations} \right)$$

- This form has some similarities to density dependent Gogny interaction. We are planning similar kind of implementation for axial code (see Chappert et al, PRC 91, 034312 (2015))
- Angular momentum projection requires a generalization of this method (density matrix no longer block-diagonal in axial case)
- (A full finite range 3N potential would probably be computationally too expensive in beyond mean-field calculations)

In collaboration with K. Bennaceur and J. Dobaczewski

Impact of time-odd part

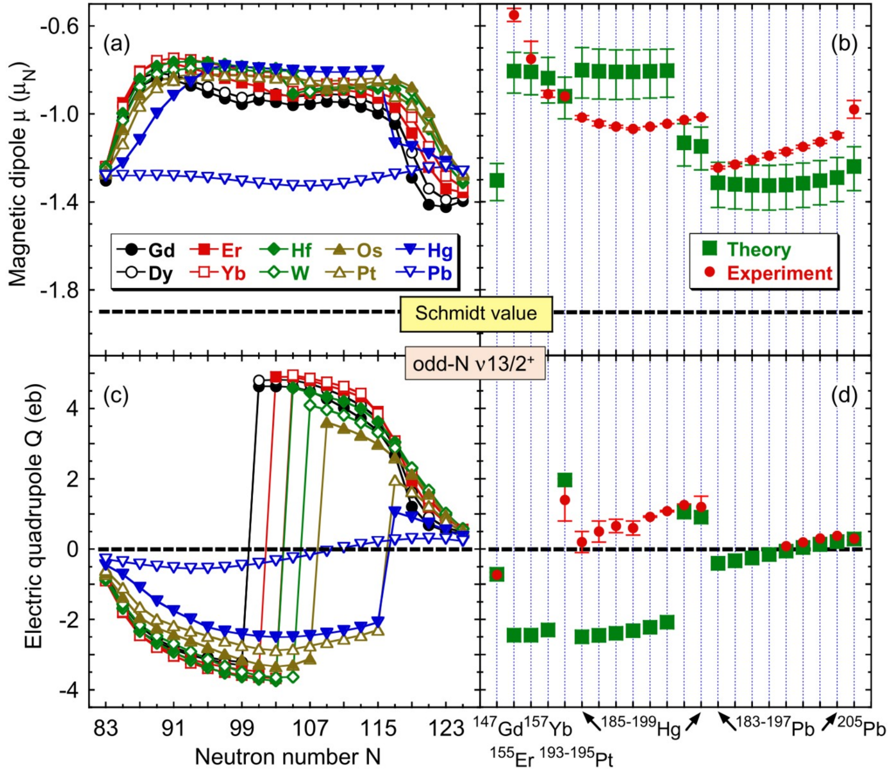
- The Skyrme EDF can be split to part constructed from time-even densities and part constructed from time-odd densities.
- Typical adjustment on considers observables sensitive on time-even part, leading to poorly constrained time-odd part of the EDF
- Some observables sensitive on time-odd part
  ⇒ can result to poor predictive quality of the EDF model
- For example, magnetic moments are sensitive to Landau parameter g'_0 (spin-spin channel)



RMS deviation and avg. deviation of magnetic moments in doubly magic nuclei ±1 particle.
From P.L. Sassarini, J. Dobaczewski, J. Bonnard, R.F. Garcia Ruiz, J. Phys. G 49, 11LT01 (2022)

Electromagnetic moments in deformed odd-A nuclei

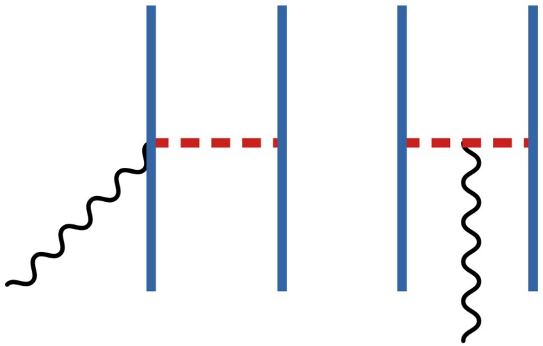
- First large-scale systemic survey of nuclear electromagnetic moments was recently conducted for odd-*A* nuclei
- Calculation done from angular momentum projected (AMP) HFB state with HFODD code
- Time-odd part of EDF from earlier work of P.L. Sassarini, et al., JPG 49, 11LT01 (2022)
- Magnetic moment sensitive to time-odd part. Could used in the future to adjust EDF parameters?
- It turned out that particle number projection has vary small impact on the results
- Projected magnetic moments can not be deduced from the unprojected ones



- AMP recently also implemented on HFBTEMP code for axial HFB state

J. Bonnard, J. Dobaczewski, G. Danneaux, M.K., Phys. Lett. B 843, 138014 (2023)

Magnetic moments: two-body currents



- In effective field theory, when going beyond LO, the electromagnetic operator attains additional contributions from two-body currents (2bc). These stem from two diagrams on right
- Recent work by T. Miyagi et al, PRL 132, 232503 (2024) shows that these improve the description of experimental magnetic moments in ab-initio calculations
- Implementation to HFBTEMP by Rui Han at Jyväskylä and to HFODD by York group
- Very first preliminary test results seems to indicate that inclusion of 2bc improves results for 39K.
- Time-odd part of the used EDF was adjusted to magnetic moments earlier without 2bc. New adjustment required
- Systematic survey needs to be done to check if they improve results

In collaboration with R. Han, B. Backes, J. Dobaczewski, H. Wibowo

Conclusions / Outlook

- The SR Skyrme EDF approach has reached its limits and new approaches are called for to improve description of nuclear properties
- Restoration of broken symmetries essential for many observables.
- The new EDF should be singularity-free for beyond mean-field calculations: Use underlying force as an EDF generator
- 3N force required
- Parameter adjustment strategy needs some thought on how to include observables which are connected to time-odd part of the EDF
- Proper Bayesian parameter uncertainty quantification should be done for EDF parameters
- A lot of applications with the new EDF (nuclear bulk properties, EM moments, spectroscopy, Schiff moment, fission, β-decays, ...)

Some open questions

- What/where is the link between the beyond mean-field EDF approach and ab-initio approach? Is there a such kind of interface?

- Can elements from ab-initio approach incorporated for an EDF intended for beyond mean-field calculations? If yes, how?

- When selecting the form of an effective interaction for EDF, what is the appropriate balance between EDF complexity and computational cost?

- Which observables are suitable for parameter adjustment of a EDF intended for beyond mean-field calculations? Impact on EDF parameter uncertainties?

- Emulators for beyond mean-field EDF calculations?

Backup slides

Angular momentum and particle number projection

- A state with good angular momentum can be obtained by using projection operator $P^J{}_{MK}$ as

$$|JM\rangle = \sum_K g_K \hat{P}^J_{MK}|\Psi\rangle\,, \quad \hat{P}^J_{MK} = \frac{2J+1}{8\pi^2}\int D^{J*}_{MK}(\Omega)\hat{R}(\Omega)\mathrm{d}\Omega$$

  Here the gauge angles are the Euler angles, Ω=(α,β,γ), *D* is the Wigner D-function, which acts as a weight function, and the rotation is done by operator

$$\hat{R}(\alpha,\beta,\gamma) = \exp(i\gamma\hat{J}_z)\exp(i\beta\hat{J}_y)\exp(i\alpha\hat{J}_z)$$

- The particle number projection operator for neutron particle number is

$$\hat{P}^N = \frac{1}{2\pi}\int_0^{2\pi} e^{i\phi(\hat{N}-N)}\mathrm{d}\phi$$

  and can be defined similarly also for proton particle number.

- In practice, these integrals are usually numerically calculated with discrete values of gauge angles
- In purely axially deformed case, the restoration of angular momentum requires only integral over β angle (integrals over α and γ are trivial).

Projected energy

- Let us assume that we have a generic gauge angle(s) *g* and a generic form of projection operator as

$$\hat{P} = \int \mathrm{d}g\, D^*(g)\hat{R}(g)$$

where *D*(g) is the weight function connected to restored symmetry group
- We can define rotated wave function as

$$|\Psi(g)\rangle = \hat{R}(g)|\Psi\rangle\,, \quad |\Psi(0)\rangle = |\Psi\rangle$$

- The energy of symmetry restored state is now given as

$$E = \frac{\langle\Psi|\hat{H}\hat{P}|\Psi\rangle}{\langle\Psi|\hat{P}|\Psi\rangle} = \frac{\int \mathrm{d}gD^*(g)\langle\Psi|\hat{H}|\Psi(g)\rangle}{\int \mathrm{d}gD^*(g)\langle\Psi|\Psi(g)\rangle} = \frac{\int \mathrm{d}gD^*(g)H(g)}{\int \mathrm{d}gD^*(g)N(g)}$$

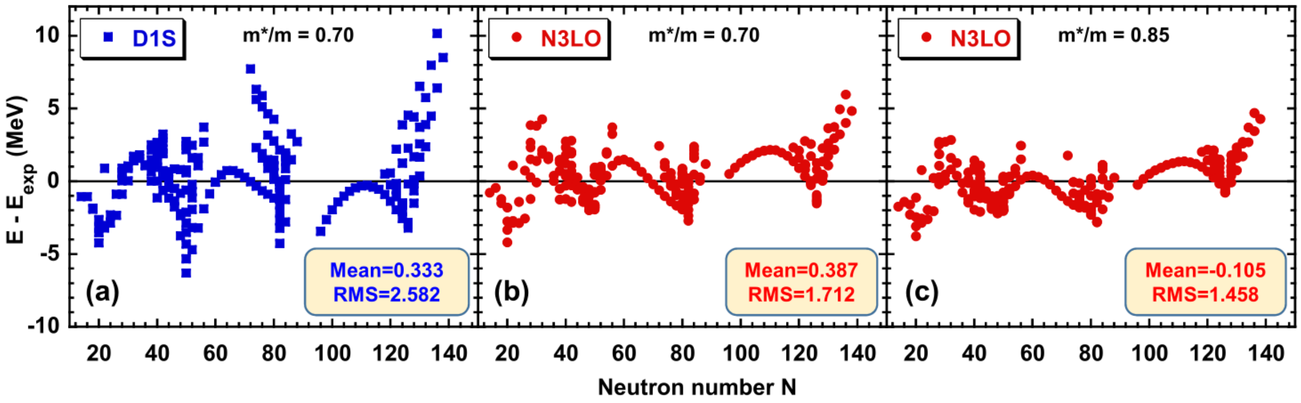
where *H*(*g*) and *N*(*g*) are the Hamiltonian kernel and the norm kernel.
- With HF or HFB case we need the density matrix to calculate the kernel. This can be obtained as

$$\rho_{ij}(g) = \langle\Psi|c_j^\dagger c_i|\Psi(g)\rangle / \langle\Psi|\Psi(g)\rangle$$

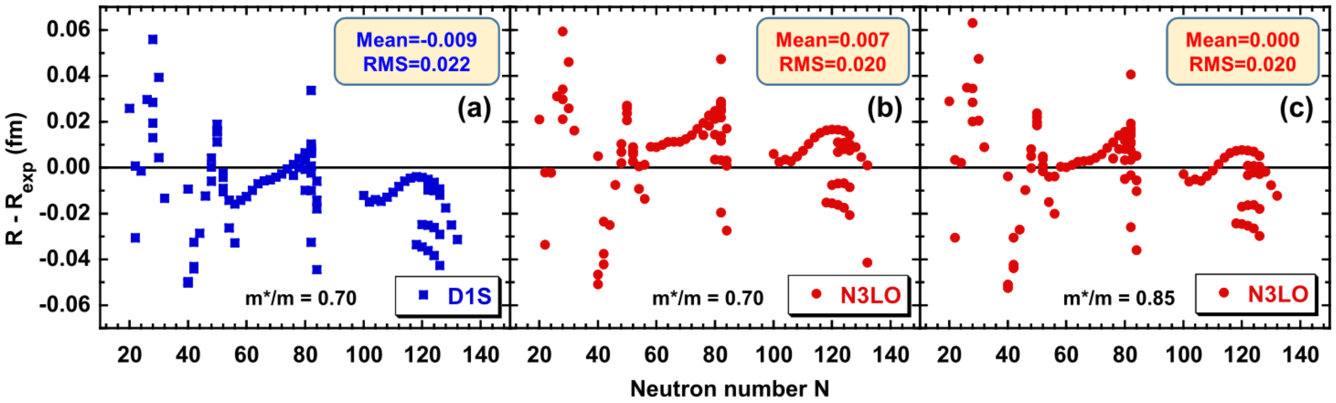
Pairing tensor can be obtained similarly. Strictly speaking, these are now transition densities. These are needed for computation of the energy kernel.

Finite range pseudopotential based EDF, second adjustment

- Nuclear mass residuals



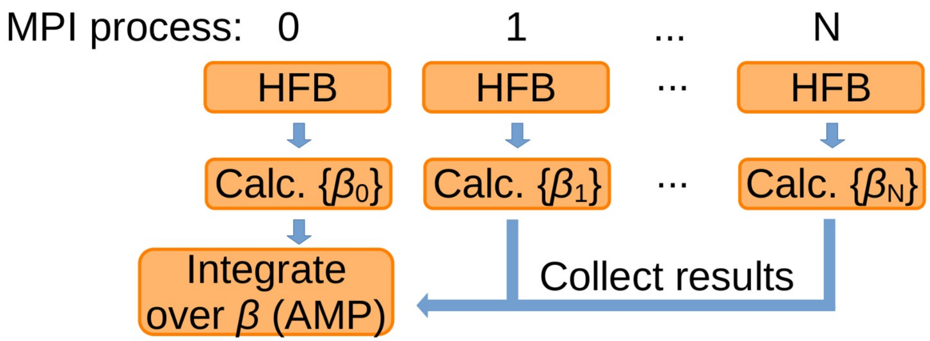
- Charge radius residuals



K. Bennaceur, J. Dobaczewski, T. Haverinen, M.K., J. Phys. G 47, 105101 (2020).

Implementation of angular momentum projection on HFBTEMP

- Angular momentum projection (AMP) for axial systems has been recently implemented on computer code HFBTEMP
- This allows computation of EM moments
- HFBTEMP is a modular HFB solver, written in modern C++
- Can break time-reversal symmetry at HFB level, to include properly all polarization effects in an odd-*A* nuclei
- The code allows to use either axial or 3D Cartesian harmonic oscillator basis
- It is also possible to implement multiple different EDFs
- Some details required for full calculations in 3D basis still needs to be implemented



- Hybrid MPI+OpenMP parallelization allows efficient use of supercomputing facilities with AMP or when computing a large set of nuclei
- Implementation of semi-contact 3N force based EDF planned in future development
- AMP in 3D Cartesian basis and configuration mixing with GCM also planned