Microscopically based energy density functionals

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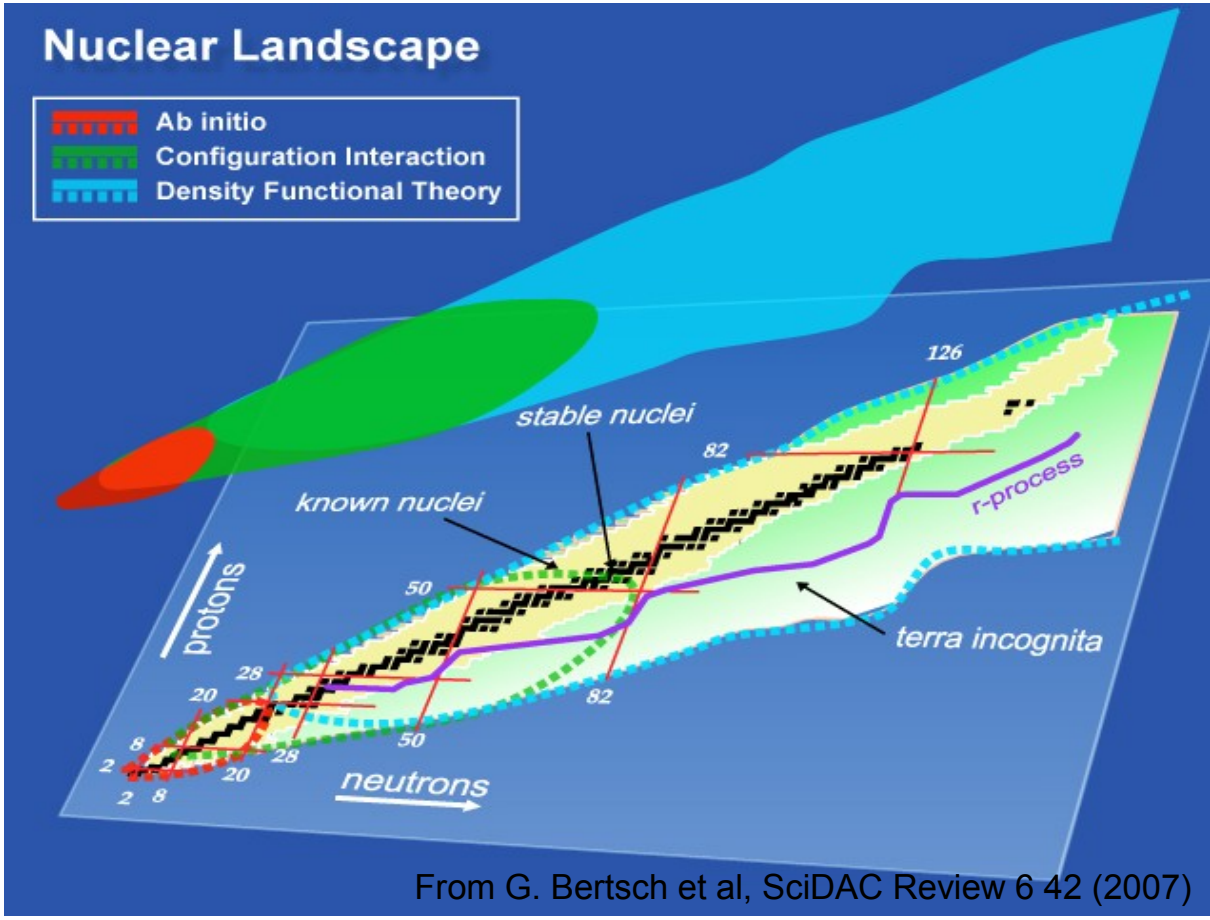
EDFs and nuclear physics

- Nuclear DFT is the only tractable microscopical theory which can be applied trough the whole nuclear chart
- Three main variants: Skyrme-like semi-local EDFs, Gogny, and relativistic mean field models
- Nuclear superfluidity taken into account with HFB or HF+BCS approach
- How to improve present EDFs?



From G. Bertsch et al, SciDAC Review 6 42 (2007)

Microscopically based energy density functionals for nuclei using the density matrix expansion: Implementation and pre-optimization

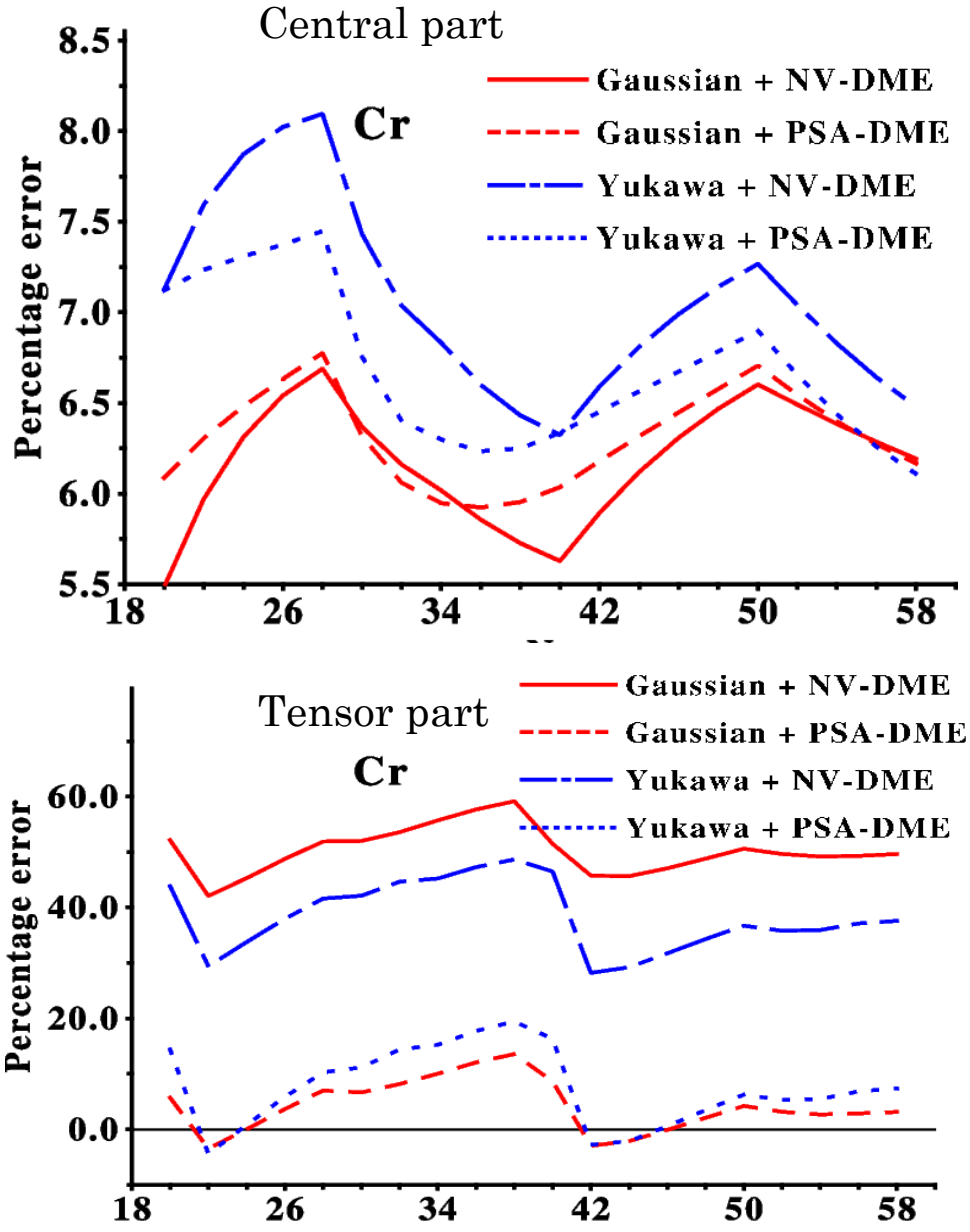
M. Stoitsov, MK, S.K. Bogner, T. Duguet,
R.J. Furnstahl, B. Gebremariam, N. Schunck
PRC 82, 054307 (2010)

Density matrix expansion

- DME can be used to construct a semi-local EDF based on some potential
- Various DME techniques: Negele-Vautherin (NV), phase-space averaging (PSA), Damped Taylor, etc.
- in DME nonlocal density matrix is expanded to sums of local densities $\mathcal{P}_n(\boldsymbol{R})$

$$\rho_t(\boldsymbol{r}_1, \boldsymbol{r}_2) \approx \sum_{n=0}^{n_{\max}} \Pi_n(kr)\ \mathcal{P}_n(\boldsymbol{R})$$

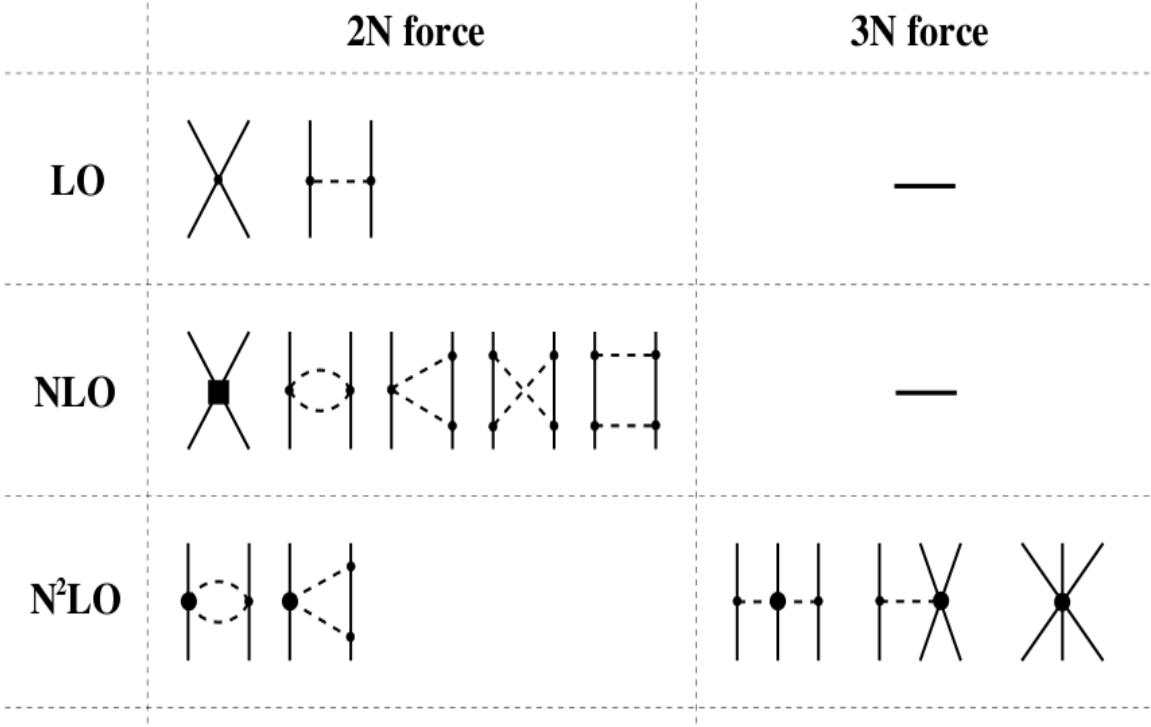
- Π-functions depend on the chosen DME technique
- for PSA see B. Gebremariam, T. Duguet, and S. K. Bogner, PRC82, 014305 (2010)
- DME expressions for energy density in different HFB solvers handled with the same fortran module.



From B. Gebremariam et al, PRC 82, 014305 (2010)

EDF from χ-potential

- With DME one can construct a semi-local energy density from the bare chiral potential
- DME functional constructed from χ-potential taken up to N2LO level
- DME done to Fock terms
- Hartree terms incorporated in Skyrme coupling constants
- 3N terms also included
- Time-even EDF constructed
- Low energy constants from E. Epelbaum, W. Glockle, and Ulf-G. Meissner, NPA747, 362 (2005)



From E. Epelbaum, arXiv:1001.3229

χ-based EDF

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(\boldsymbol{r}) + \mathcal{H}_1(\boldsymbol{r}) + \mathcal{H}_2(\boldsymbol{r})$$

$$\begin{aligned}\mathcal{H}_t(\boldsymbol{r}) = &\left[C_{t0}^{\rho^2} + C_{tD}^{\rho^2}\rho_0^{\gamma} + g_t^{\rho^2}(u) + \rho_0 h_t^{\rho^2}(u)\right]\rho_t^2 \\ &+ \left[C_t^{\rho\tau} + g_t^{\rho\tau}(u) + \rho_0 h_t^{\rho\tau}(u)\right]\rho_t\tau_t \\ &+ \left[C_t^{\rho\Delta\rho} + g_t^{\rho\Delta\rho}(u) + \rho_0 h_t^{\rho\Delta\rho}(u)\right]\rho_t\Delta\rho_t \\ &+ \left[C_t^{\rho\nabla J} + g_t^{\rho\nabla J}(u) + \rho_0 h_t^{\rho\nabla J}(u)\right]\rho_t\nabla J_t \\ &+ \left[C_t^{J^2} + g_t^{J^2}(u) + \rho_0 h_t^{J^2}(u)\right]J_t^2\end{aligned}$$

$$\begin{aligned}\mathcal{H}_2(\boldsymbol{r}) = &\rho_1 h_{10}^{\rho\tau}(u)\rho_1\tau_0 + \rho_1 h_{10}^{\rho\Delta\rho}(u)\rho_1\Delta\rho_0 \\ &+ \rho_1 h_{10}^{J^2}(u)J_1J_0 + \rho_1 h_{10}^{\rho\nabla J}(u)\rho_1\nabla J_0\end{aligned}$$

- Obtained EDF resembles Skyrme-like EDF with density dependent coupling constants
- 2N terms contribute to g(u) terms
- 3N terms contribute to h(u) terms
- Obtained EDF is isospin symmetric
- Coupling constants C needs to be optimized to experimental data

Example of g(u) function at LO:

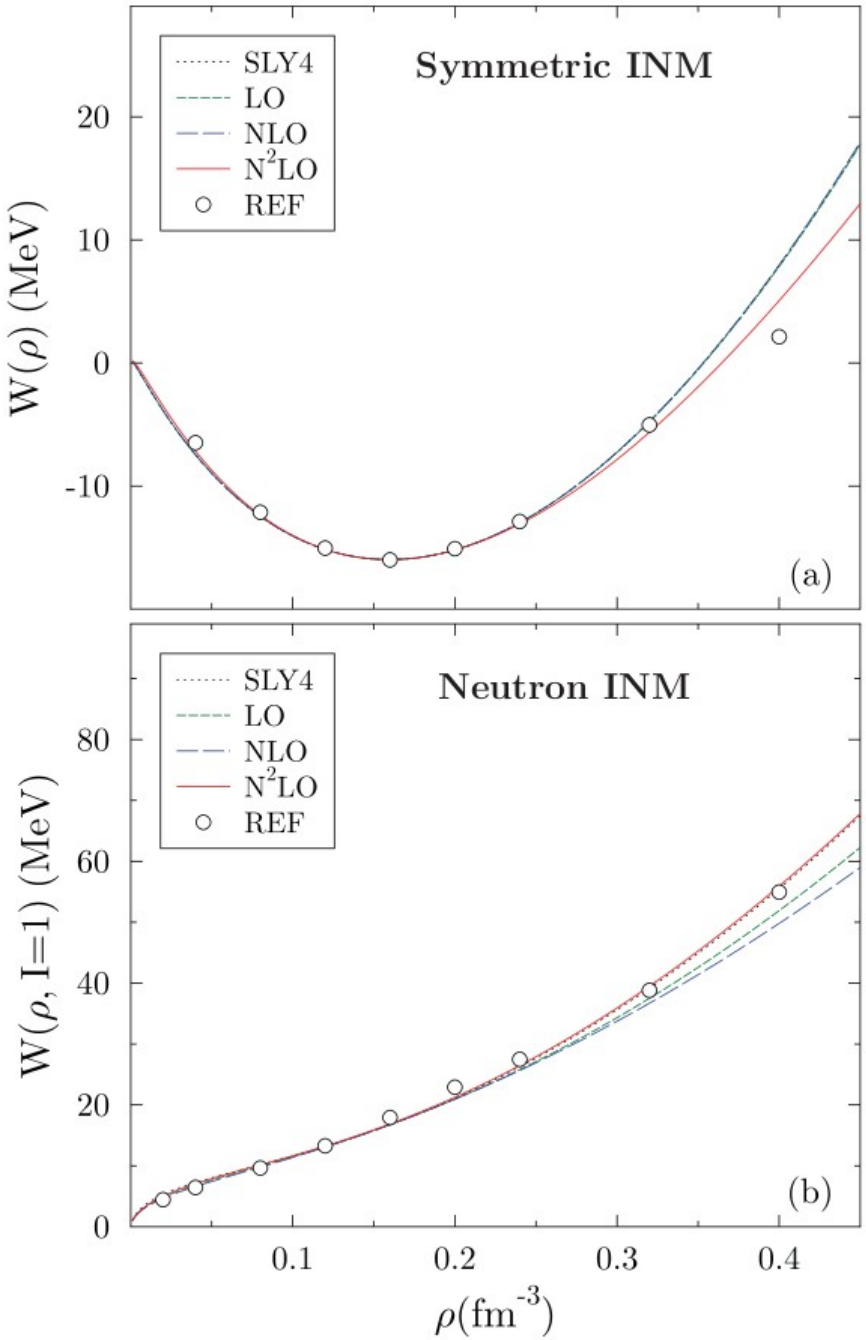
$$g(u)|_{\mathrm{LO}} = \alpha_0^g + \beta_0^g \log(1+4u^2) + \gamma_0^g \arctan(2u)$$

α, β, and γ are rational polynomials of u.

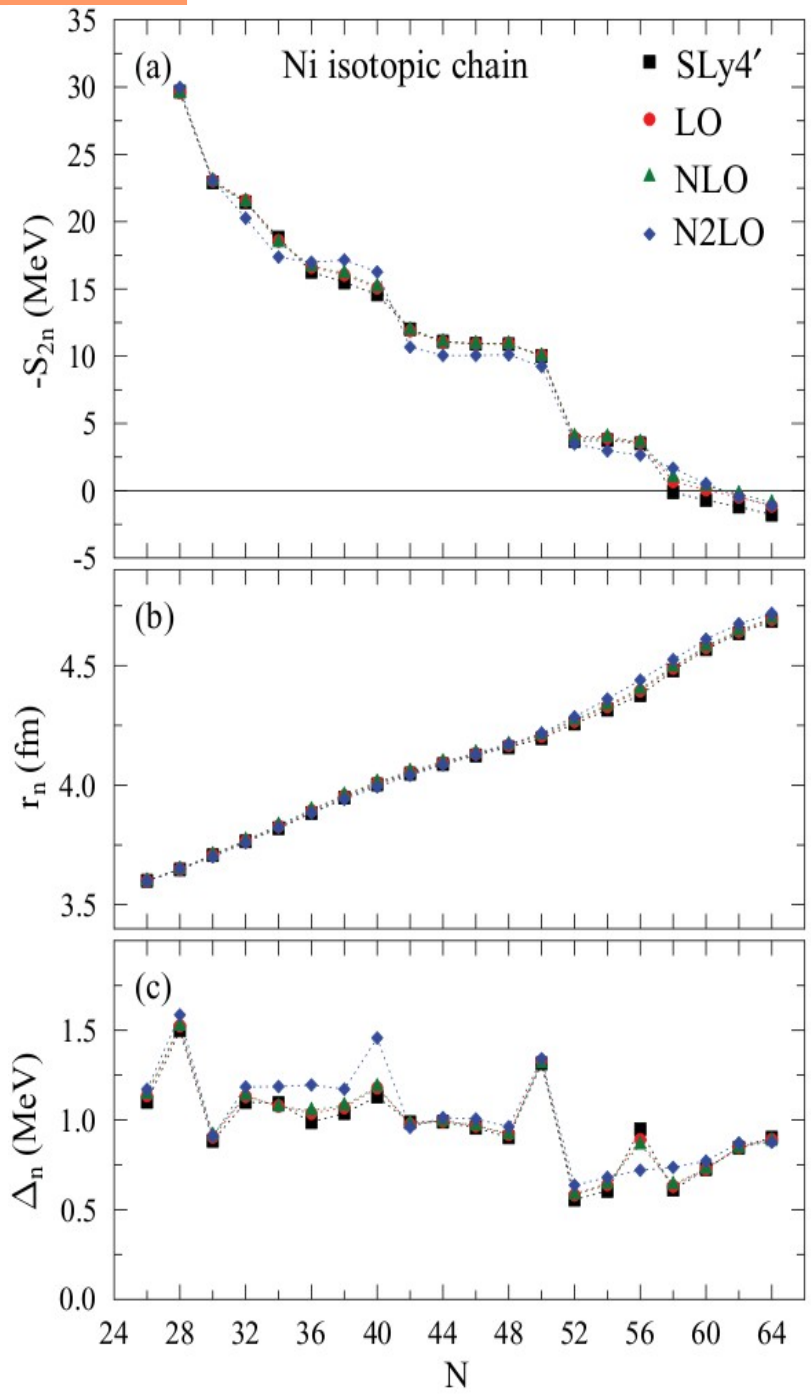
Pre-Optimization of χ-based EDF

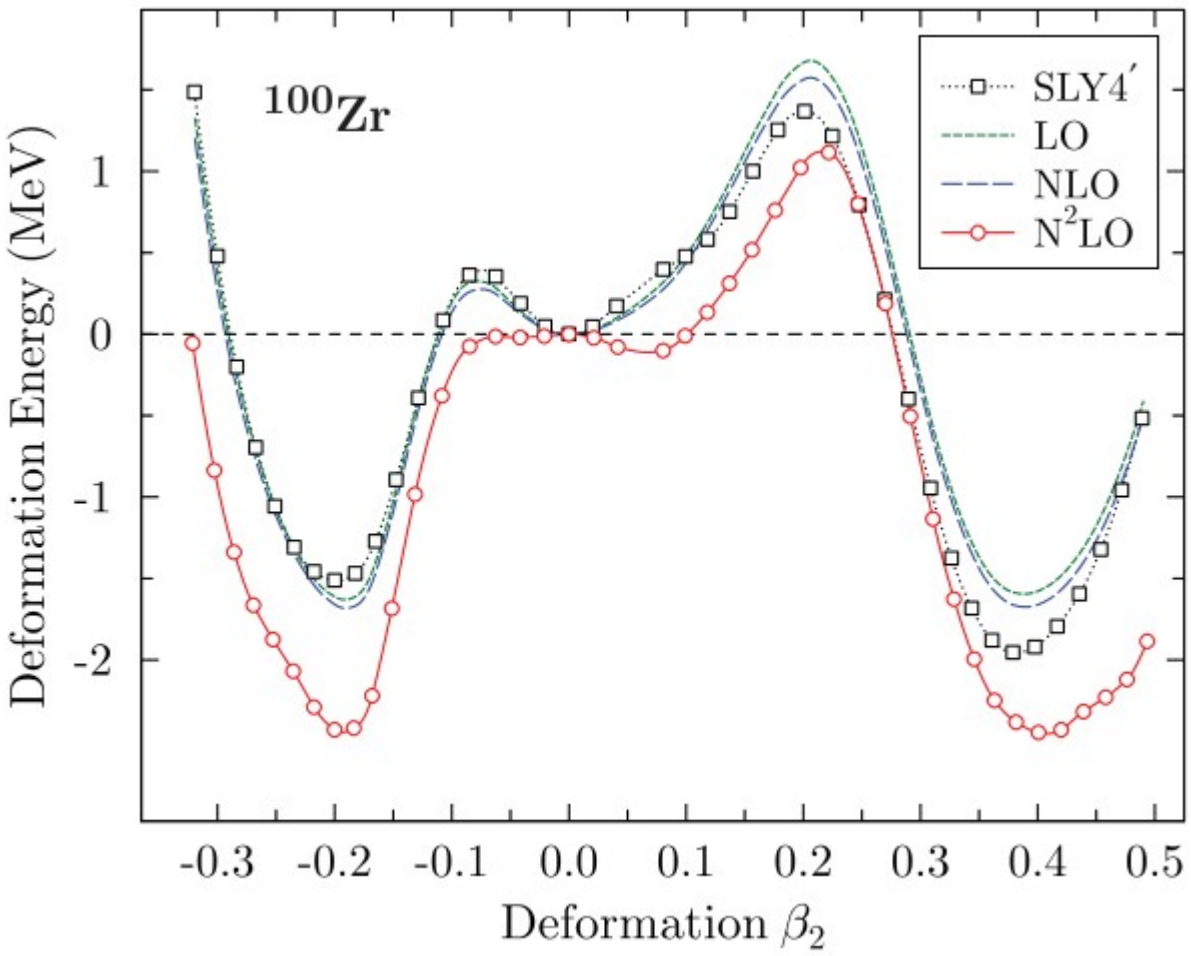
- Volume part of the EDF was taken to from infinite nuclear matter properties of SLY4 with small modifications to the asymmetric INM parameters
- Surface coupling constants and pairing part were optimized to the masses and OEM data of UNEDF0 dataset
- Optimization improved total χ^2 compared to basic Skyrme-like EDF

	SLy4	SLy4′	LO	NLO	N^{2}LO
χ^2	12.5002	2.1235	1.837	1.7662	1.7884
$RMSD(E)$	7.008	2.6931	2.5539	2.5143	2.590
$RMSD(\Delta_n)$	0.1297	0.0828	0.0587	0.0554	0.0476
$RMSD(\Delta_p)$	0.094	0.0988	0.0902	0.0866	0.0706



Some results

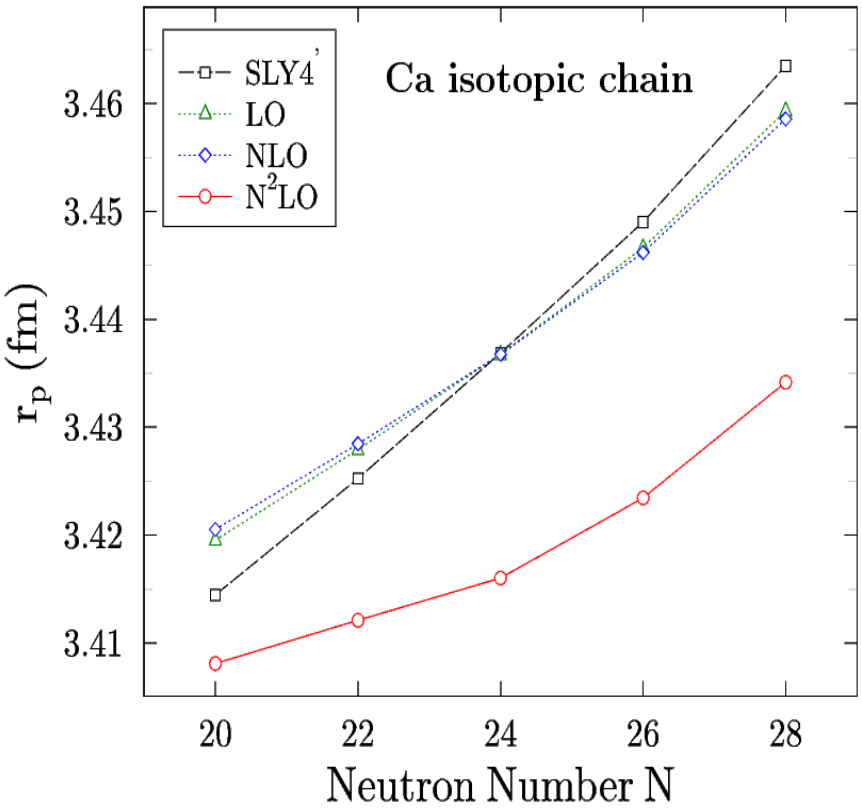




- Pre-optimized DME functional gives roughly similar results compared to Skyrme. Some details differ

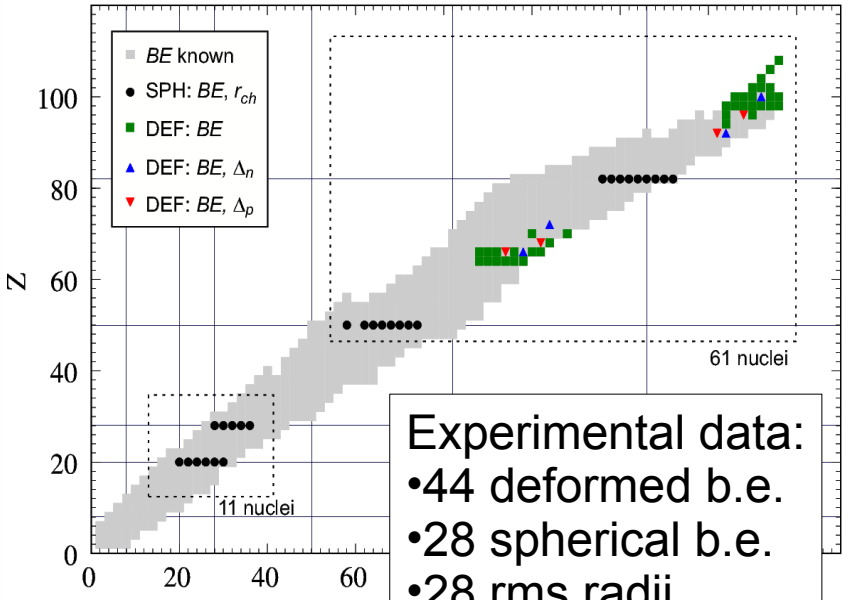
Some results and outlook for optimization

- Skyrme-like EDFs usually work rather well (but not perfectly) in many cases $\Rightarrow$ results of χ-based EDF should not deviate much from Skyrme
- χ-based DME EDF is expected to improve Skyrme results
- In order to make conclusive comparison of Skyrme-like EDF and χ-based DME EDF one needs to compare properly optimized functionals
- Use UNEDF procedure for EDF optimization



EDF optimization with UNEDF procedure

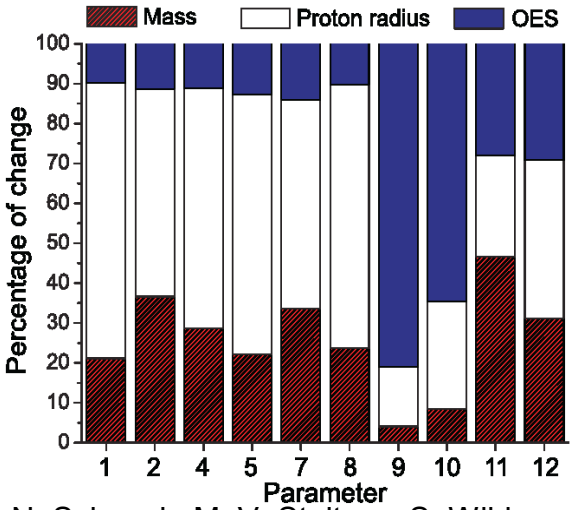
- UNEDF0 optimization



Experimental data:
- 44 deformed b.e.
- 28 spherical b.e.
- 28 rms radii
- 8 oes energies

POUNDerS-algorithm

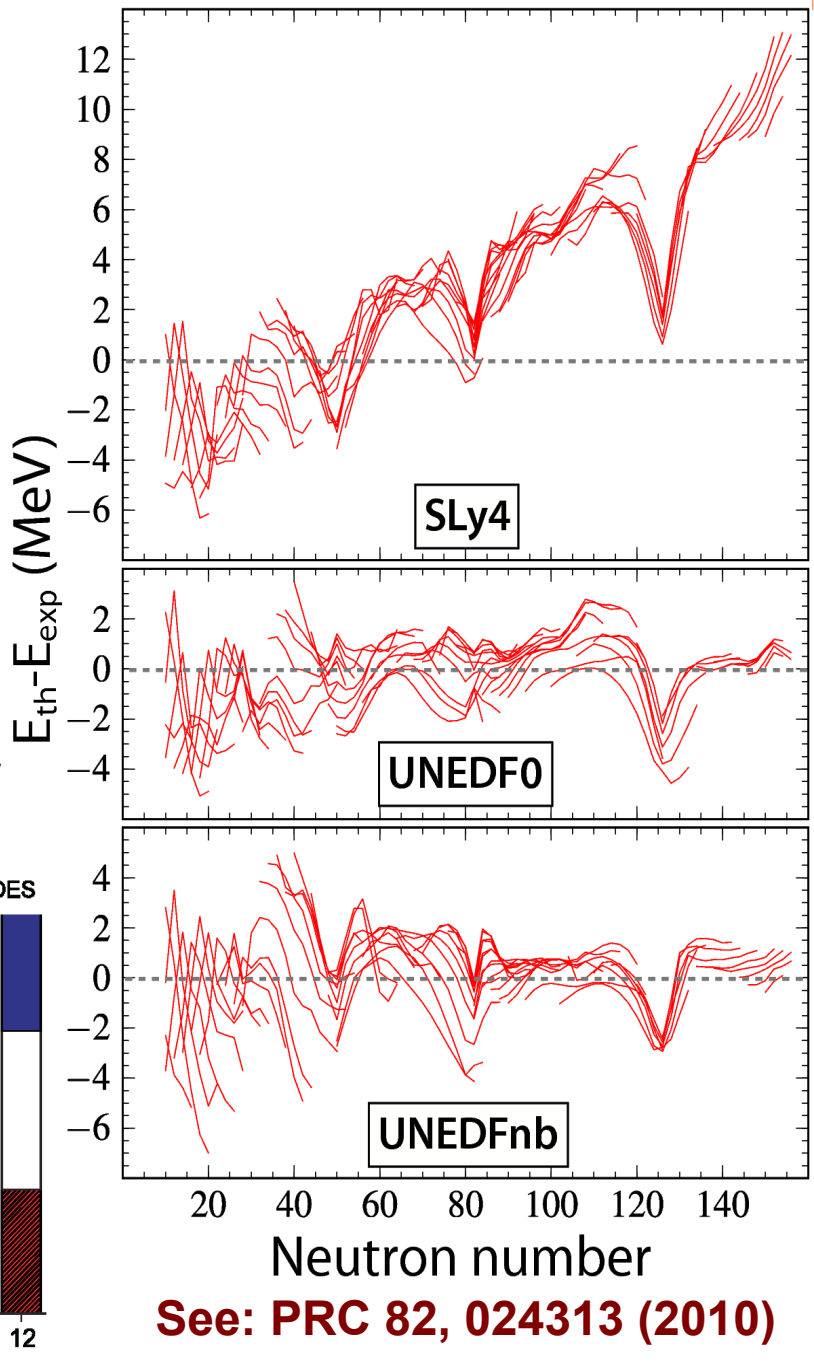
- Full correlation analysis done for the optimum



- Optimization of Skyrme-like ED with respect of 12 parameters:

$$\rho_c, E^{NM}/A, K^{NM}, a_{sym}^{NM}, L_{sym}^{NM}, M_s^{-1}$$
$$C_0^{\rho\Delta\rho}, C_1^{\rho\Delta\rho}, V_0^n, V_0^p, C_0^{\rho\nabla J}, C_1^{\rho\nabla J}$$

- Optimization carried with axial-symmetric code HFBTHO (deformed HFB)

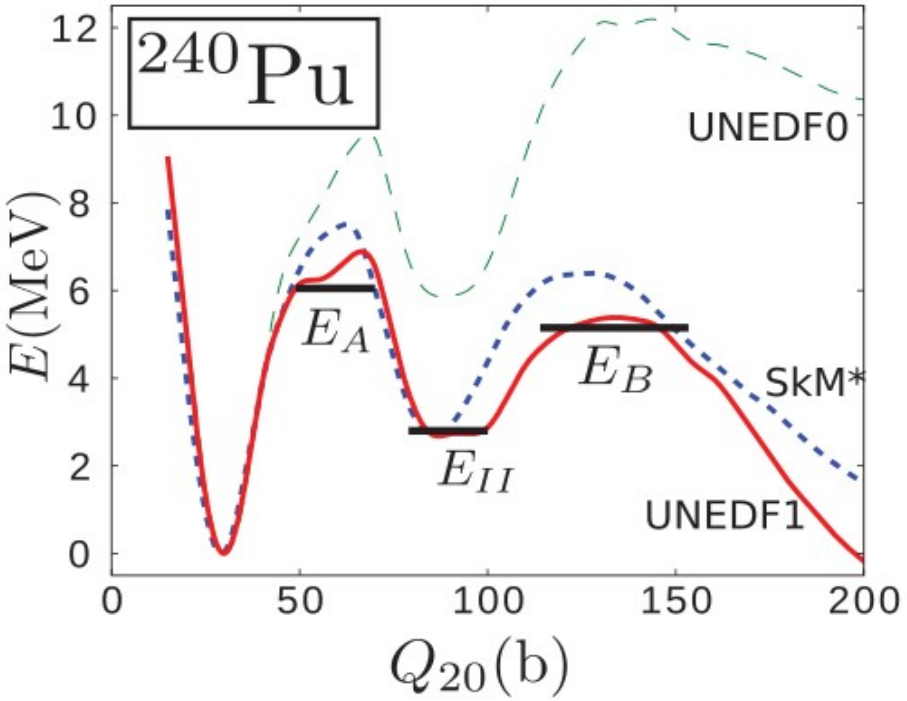


See: PRC 82, 024313 (2010)

MK, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild

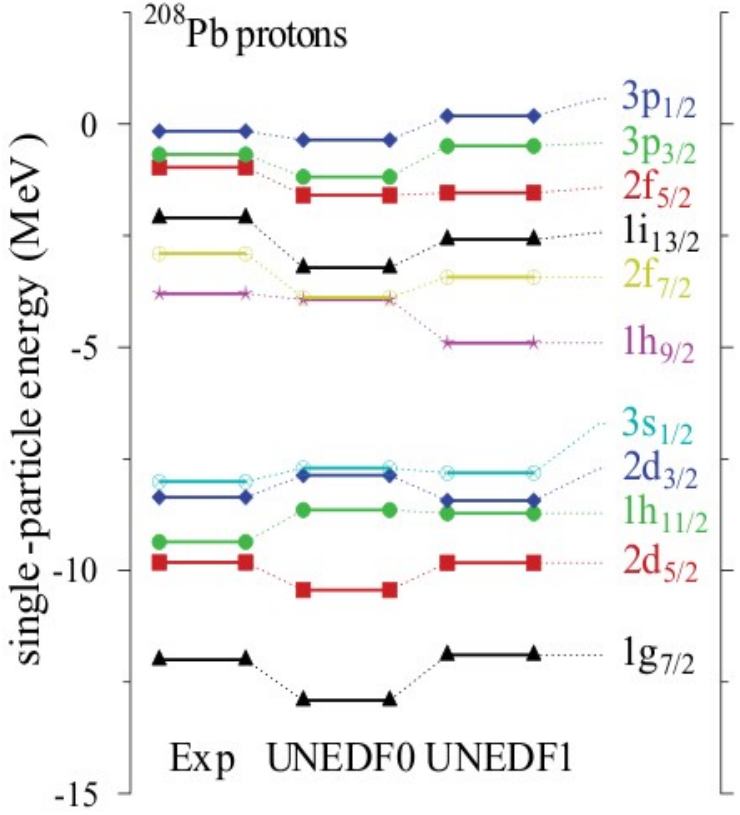
EDF optimization with UNEDF procedure

- UNEDF1 optimization:
- Database expanded with 4 fission isomer excitation energies and 3 masses in actinide region
- Improves description of fission barriers
- Sensitivity analysis done like with UNEDF0 to obtain correlations and parameter uncertainties



UNEDF1: MK, J. McDonnell, W. Nazarewicz, P.-G. Reinhard, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, PRC 85, 024304 (2012)

- Future EDF optimization:
- New data to be included on single-particle levels, giant resonances, neutron droplets, etc. for optimization procedure
- Optimization of χ-based EDF
- Sensitivity analysis essential tool to quantify uncertainties and predictive power



Implementation to EDF solvers

- Skyrme EDF is constructed from bilinear terms of density matrices and their derivatives up to the 2nd order
- Each term multiplied by a constant coupling constant (except C^{ρ})

$$H_t^{even}(r) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla J_t + C_t^{J}J_t^2$$

$$C_t^{\rho} = C_{t0}^{\rho} + \rho_0^{\gamma}C_{tD}^{\rho} \quad , \quad t = 0,1$$

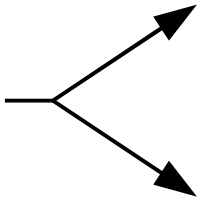
- Generalize time-even H(r) to density dependent coupling constants U[ρ]

$$H_{tt'}^{even}(r) = U_{tt'}^{\rho\rho}\rho_t\rho_{t'} + U_{tt'}^{\rho\tau}\rho_t\tau_{t'} + U_{tt'}^{\rho\Delta\rho}\rho_t\Delta\rho_{t'} + U_{tt'}^{\nabla\rho\nabla\rho}\nabla\rho_t\cdot\nabla\rho_{t'}$$
$$+ U_{tt'}^{\rho\nabla J}\rho_t\nabla J_{t'} + U_{tt'}^{J\nabla\rho}J_t\cdot\nabla\rho_{t'} + U_t^{JJ}J_tJ_{t'}$$

Implementation to EDF solvers

- Main idea is to separate details of EDF and HFB solver
- All functional details coded in fortran module UNEDF: The same module for different HFB solvers
- At the moment HFBRAD and HFBTHO works with the module

UNEDF DME module (f90)
- contains DME and Skyrme functionals
- calculates numerical values of CCs and their derivatives
- inm. properties included
- i/o for functional parameters



HFBTHO
- HO basis
- axial-symmetry

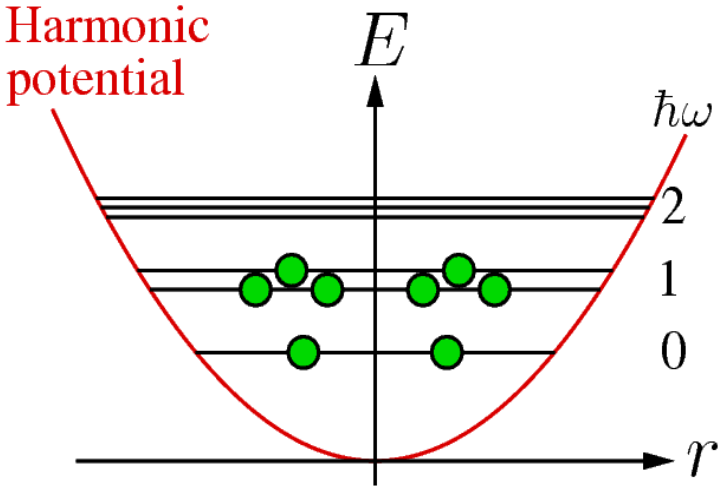
HFBRAD
- coordinate space
- spherical symmetry

```
!
! === PUBLIC VARIABLES ===
!
! Use pointers to prevent conflicts with UNEDF public variabes
! Example: Use UNEDF, pr=>my_pr, ipr=>my_ipr, Crho=>my_Crho ...
!
Integer, Parameter, Public :: pr=Kind(1.0D0), ipr=Kind(1)                    ! to set the pre
Logical, Public :: use_charge_density, use_cm_cor
Real(pr), Public, Dimension(0:3,0:7) :: Urhorho,Urhotau,UrhoDrho,Unablarho   ! ph DME amplitu
Real(pr), Public, Dimension(0:3,0:7) :: UJnablarho,UrhonablaJ,UJJ
Real(pr), Public, Dimension(0:3,0:7) :: Urhorhopr                            ! pp amplitudes
Real(pr), Public, Dimension(0:1) :: UEnonstdr,UFnonstdr,URnonstdr            ! Other amplitud
Real(pr), Public :: hbzero,sigma,e2charg                                     ! hbr^2/2m, DD s
Real(pr), Public, Dimension(0:1) :: Crho,Cdrho,Ctau,CrDr,CrdJ,CJ,CpV0,CpV1  ! basic coupling
Real(pr), Public :: E_NM,K_NM,SMASS_NM,RHO_NM,ASS_NM,LASS_NM,VMASS_NM,P_NM,KA_NM
Real(pr), Public :: CHrho                                                    ! Crho(0) from t
Logical, Public :: use_DME3N_terms,use_j2terms
Integer(ipr), Public :: DMEorder,DMElda
!
! === PRIVATE VARIABLES ===
!
Real(pr), Private, Dimension(0:1) :: nuCrho,nuCdrho,nuCtau,nuCrDr            ! basic coupling
Real(pr), Private, Dimension(0:1) :: nuCrdJ,nuCJ,nuCpV0,nuCpV1               !
Real(pr), Private :: t0,t1,t2,t3,x0,x1,x2,x3,b4,b4p,te,to
Real(pr), Private :: nuLambda,nufpi                                          ! parameters ass
```

Neutron droplets in DFT

Neutron droplets and DFT

- inhomogeneous neutron matter can be studied theoretically in some trapping potential
- DFT originally formulated by Hohenberg-Kohn for systems in external potential. It states that there exists a functional of density which produces exact MB energy
- in Kohn-Sham scheme the MB correlation energy is accounted by the interaction-correlation function
- neutron droplets can be used to study and compare different many-body methods
- ab-initio calculations could be used as a pseudo-data for EDF optimization

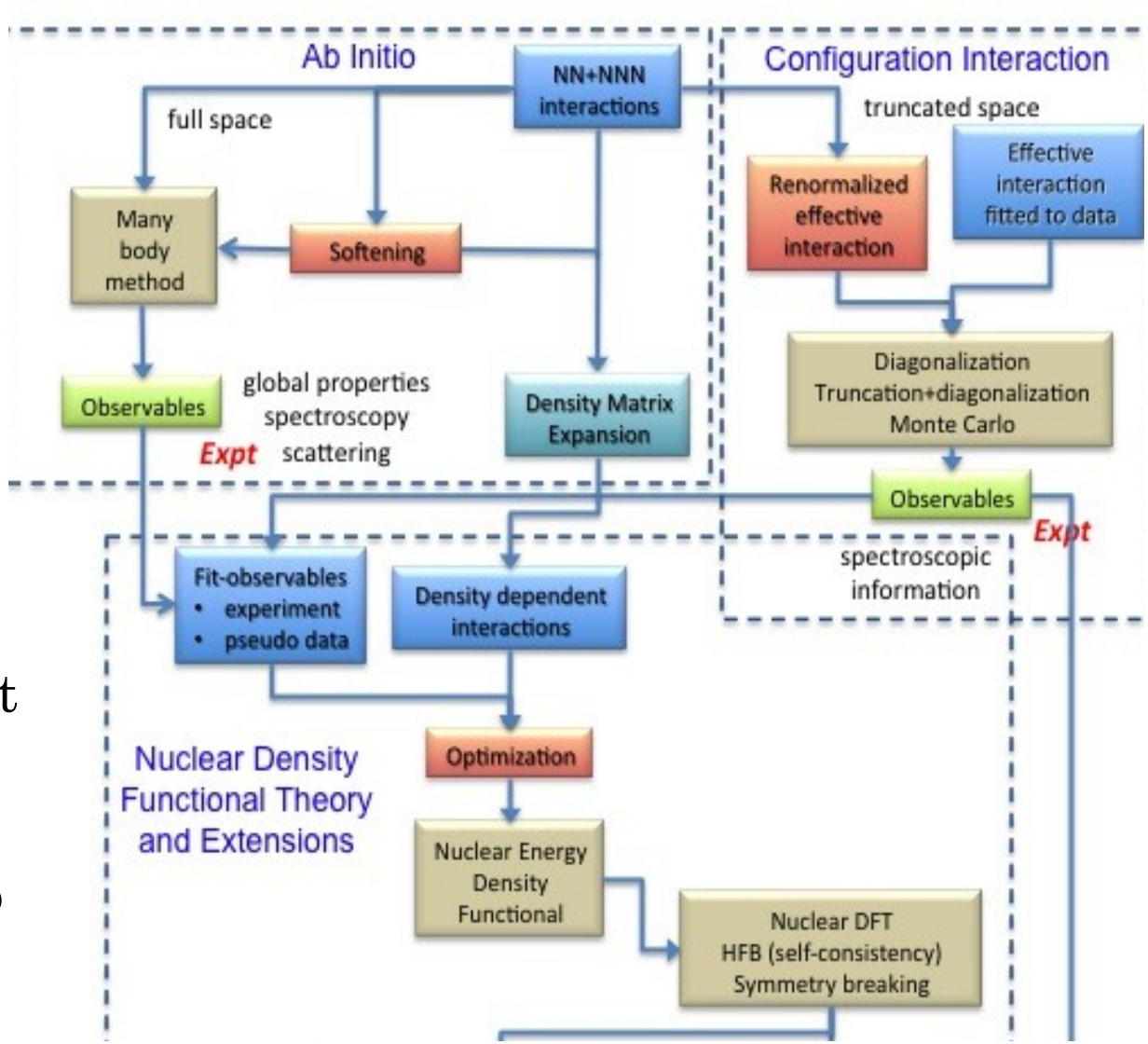


Testing the density matrix expansion against ab initio calculations of trapped neutron drops

S.K. Bogner, R.J. Furnstahl, H. Hergert,
MK, P. Maris, M. Stoitsov, and J.P. Vary,
PRC 84, 044306 (2011)

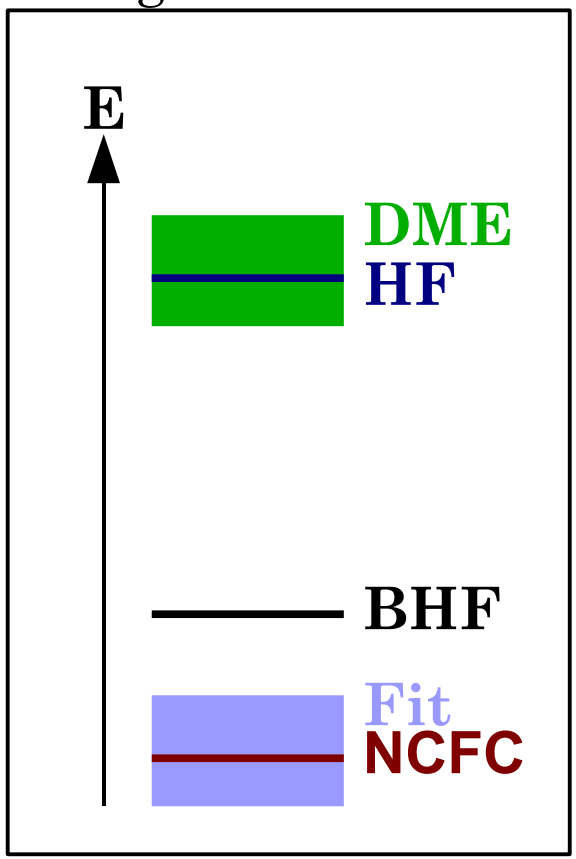
Neutron droplets and DFT

- the validity of DME techniques needs to be tested for microscopically based EDFs
- bare DME EDF should produce results which are close to the exact HF
- bare DME EDF lacks the MB correlations. It must be supplemented by some mechanism to produce exact MB results
- neutron droplets provide a controllable environment to test DME and it's supplementation against various MB methods



Comparison of different many body methods

Expected energies



- Minnesota potential (NPA286, 53 (1977)) provides a simple test case for DME
- N=8 and N=20 systems considered
- exact MB results from NCFC calculations
- NV and PSA DME applied to potential to produce semi-local EDF
- Additional correlations introduced from BHF calculations on infinite neutron matter (INM)
- the ratio of HF and BHF results in INM is a smooth function of density, $f(k_F) \rightarrow$ scale the DME functional with $f(k_F)$. This is denoted as BHF
- second option is to include BFH correlations by adding contact part to the EDF. Volume part was fitted to BHF INM and surface coupling constant to NCFC total energies. This is denoted as Fit.
- BHF and Fit expected to be close to NCFC results

Comparison of NV and PSA DME to HF

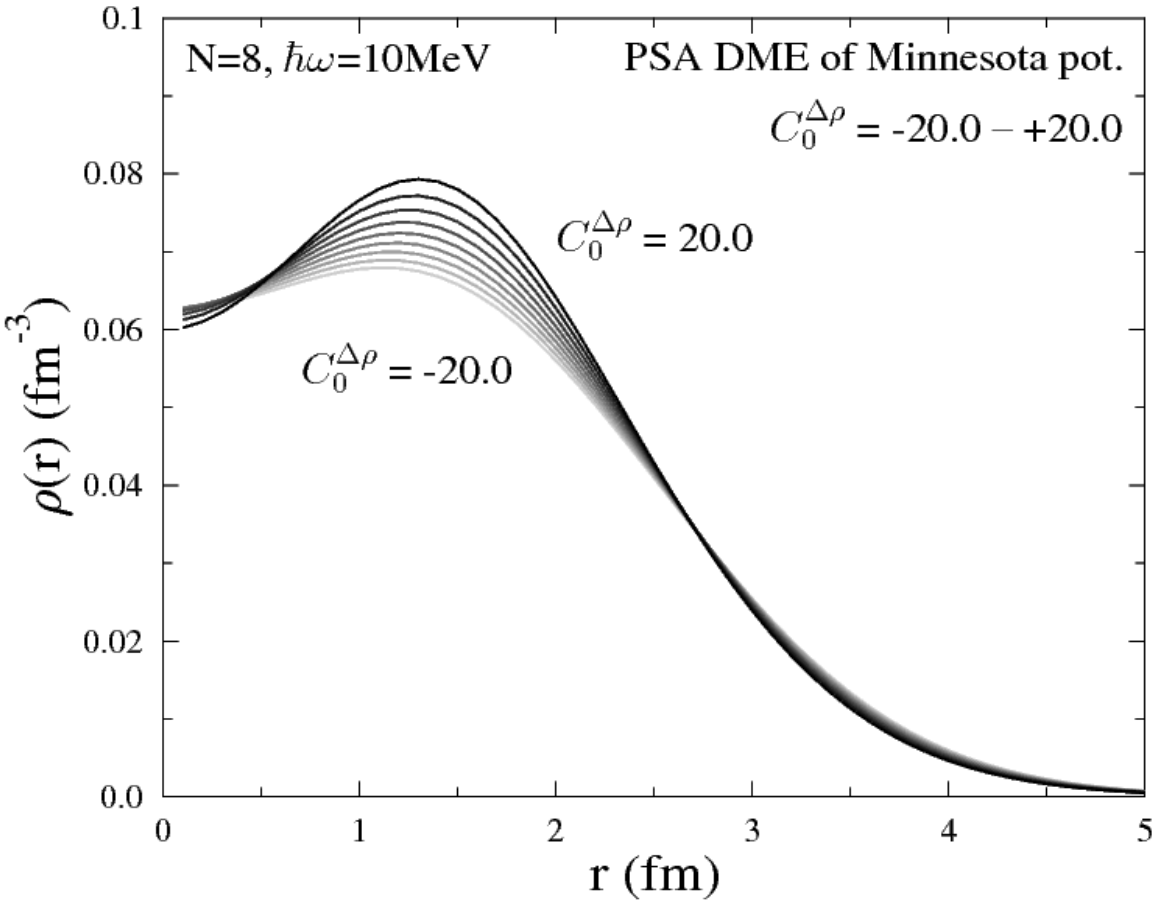
- DME can be applied to the Fock term, or on both Hartree and Fock terms
- PSA with exact treatment of Hartree term provides closest results to exact HF
- DME energies calculated from exact HF densities are almost identical to self consistent DME energies

Difference in total energy compared to exact HF in MeV

		HF/NV			HF/PSA		
N	$\hbar\Omega$	NV	NT	exact	PSA	NT	exact
8	3	0.1	0.2	0.1	0.0	0.1	0.0
8	5	0.4	0.8	0.4	−0.1	0.6	0.2
8	10	2.1	5.1	2.0	−1.7	4.1	0.9
8	15	4.2	12.9	4.6	−7.1	10.8	2.1
8	20	6.0	24.2	7.7		20.9	3.4
20	3	0.5	0.8	0.6	−0.1	0.4	0.2
20	5	1.8	3.4	2.3	−1.0	2.0	0.9
20	10	5.9	18.5	11.0	−14.0	12.0	3.9
20	15	3.8	44.3	22.7		31.6	7.9
20	20	−17.8	80.0	34.8		61.3	12.5

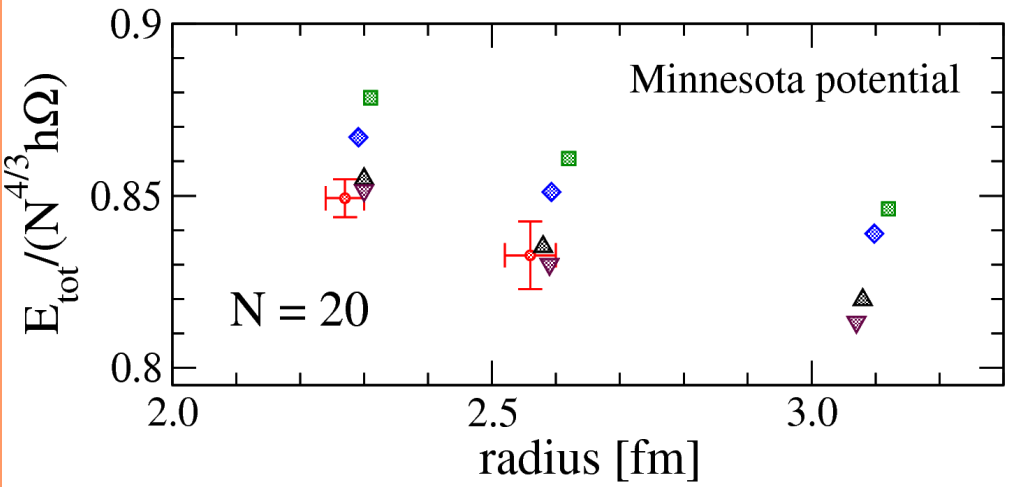
Optimization of surface coupling constant

- Volume part of the functional was fixed to produce INM properties of BHF calculations
- Surface coupling constant $C^{\Delta\rho}$ was optimized to total energies of NCFC calculations by using theoretical error bars as a weights
- Simple RMS optimization to E_{tot} of NCFC gives almost the same result

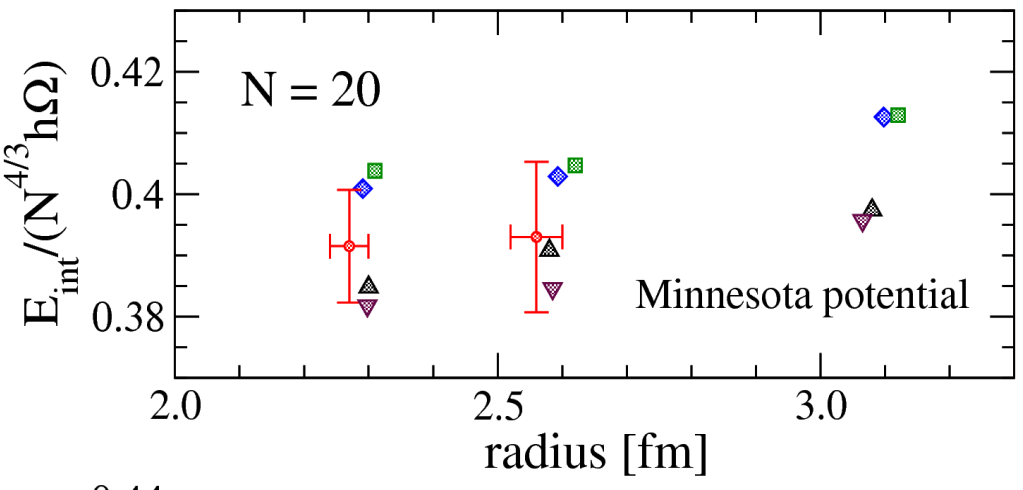


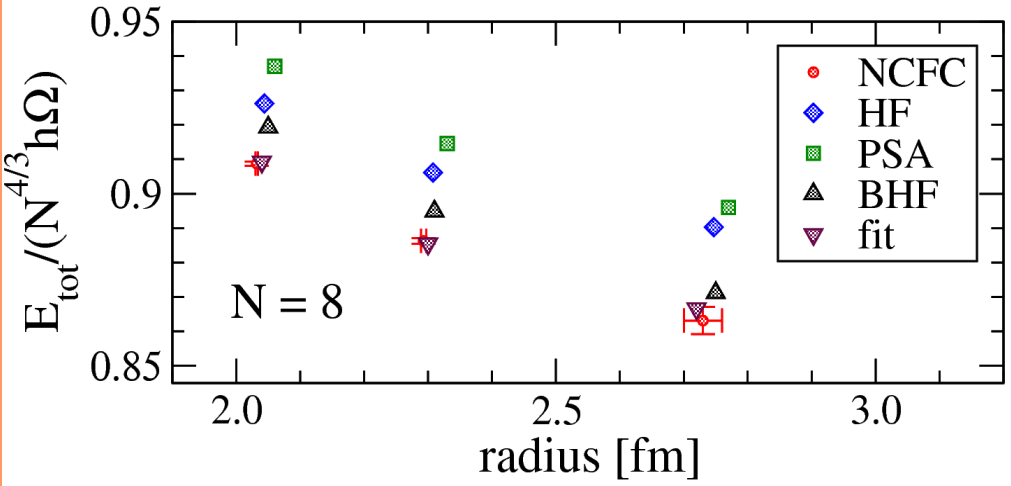
DFT and NCFC results compared

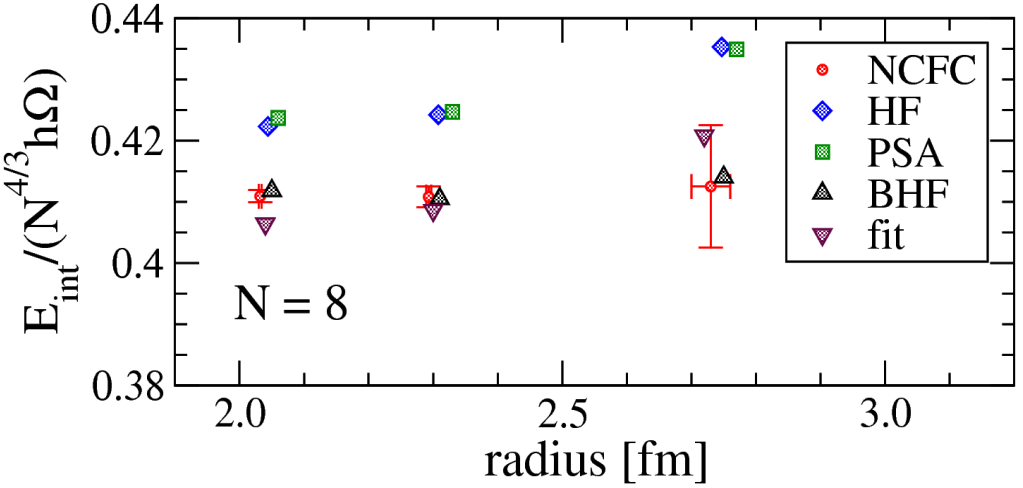
Total energies



Internal energies

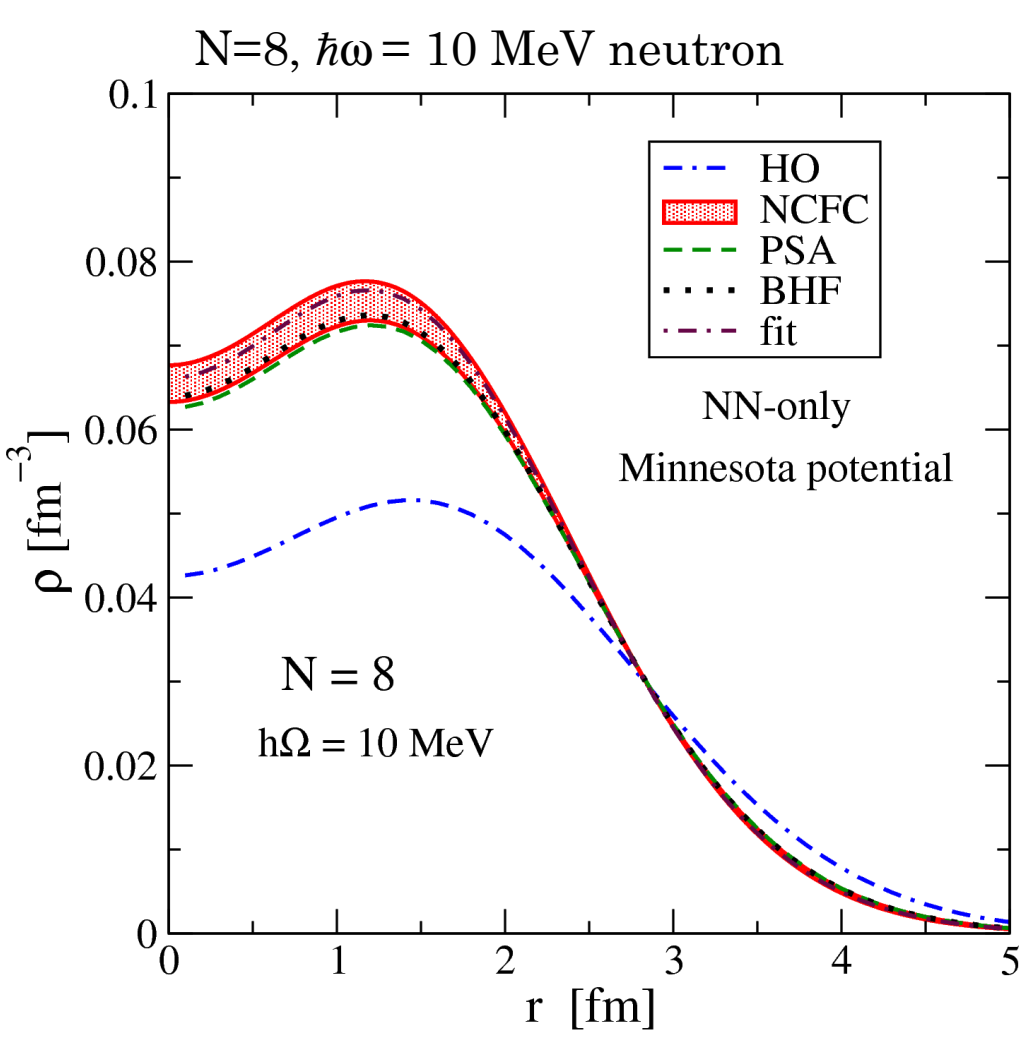


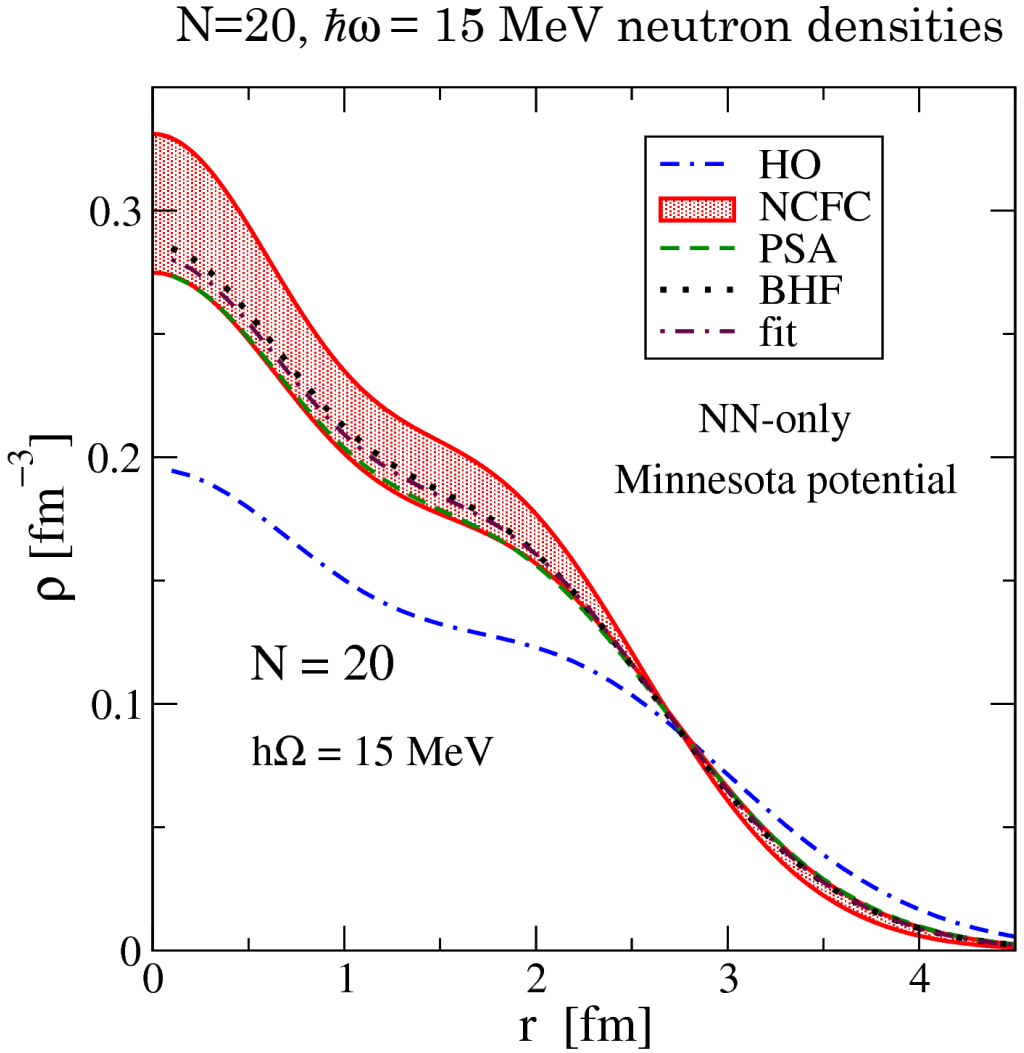




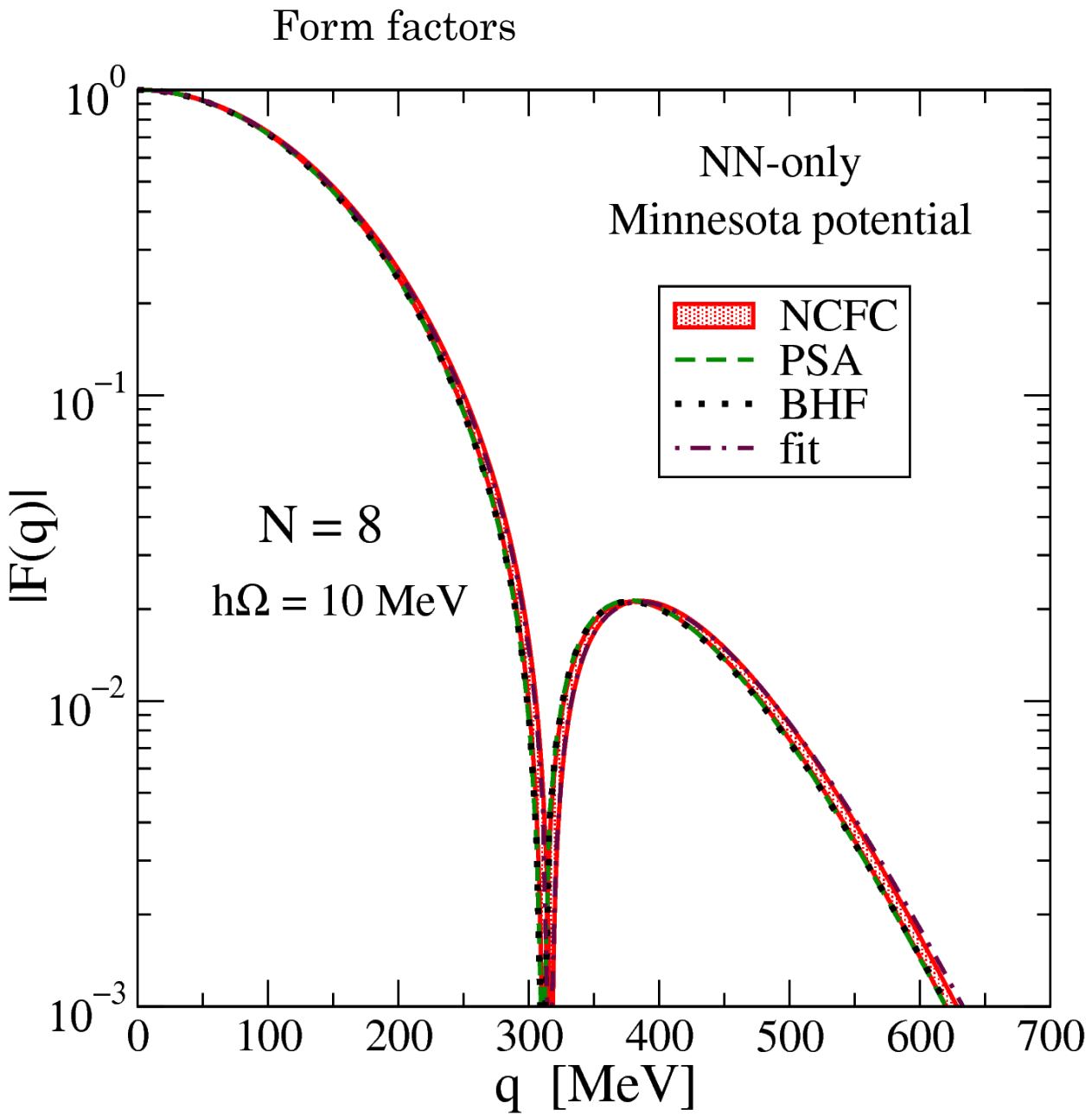
$\hbar\omega = 20,15,10$ MeV (from left to right in figures)

DFT and NCFC results compared

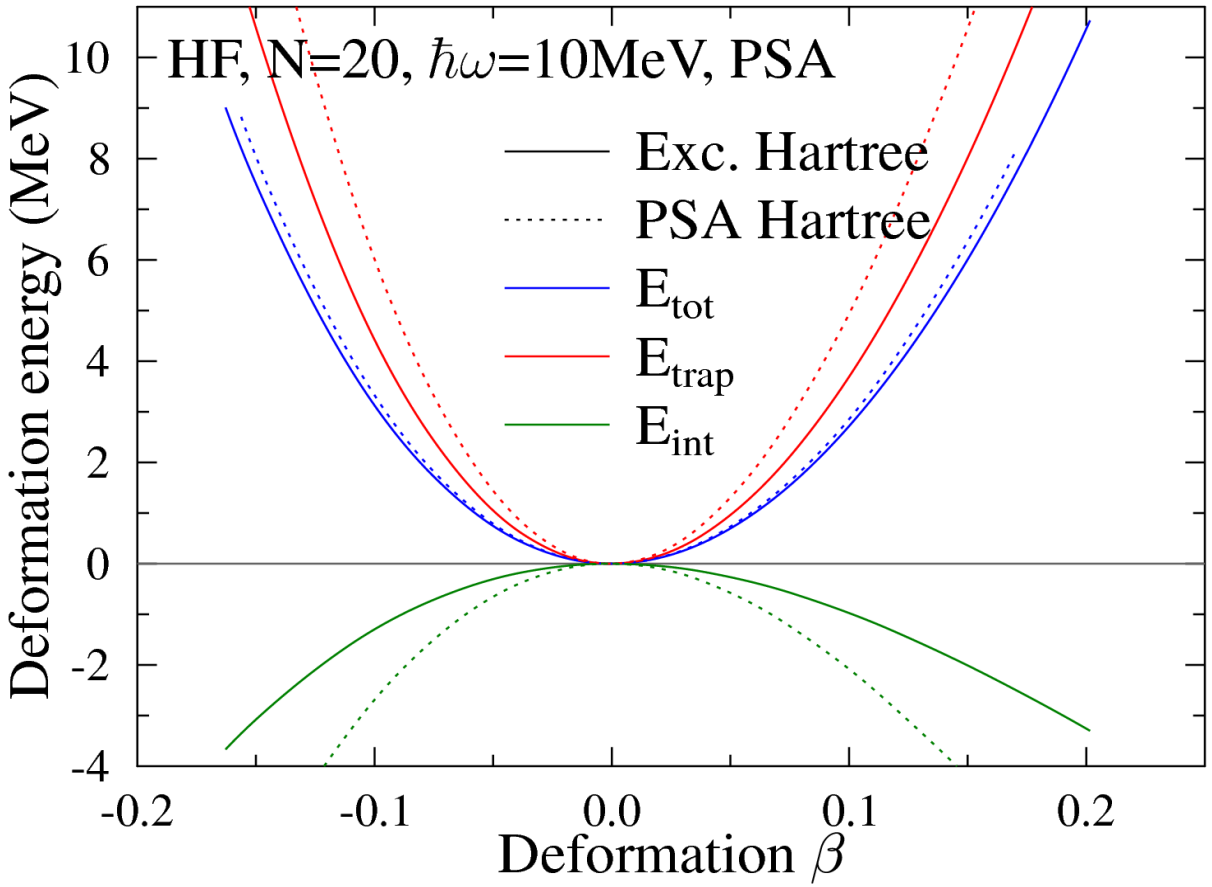




DFT and NCFC results compared



Deformation



- By imposing a constraint for quadrupole deformation, one can study deformation energy
- Spherical external potentials give the minimum energy for spherical densities

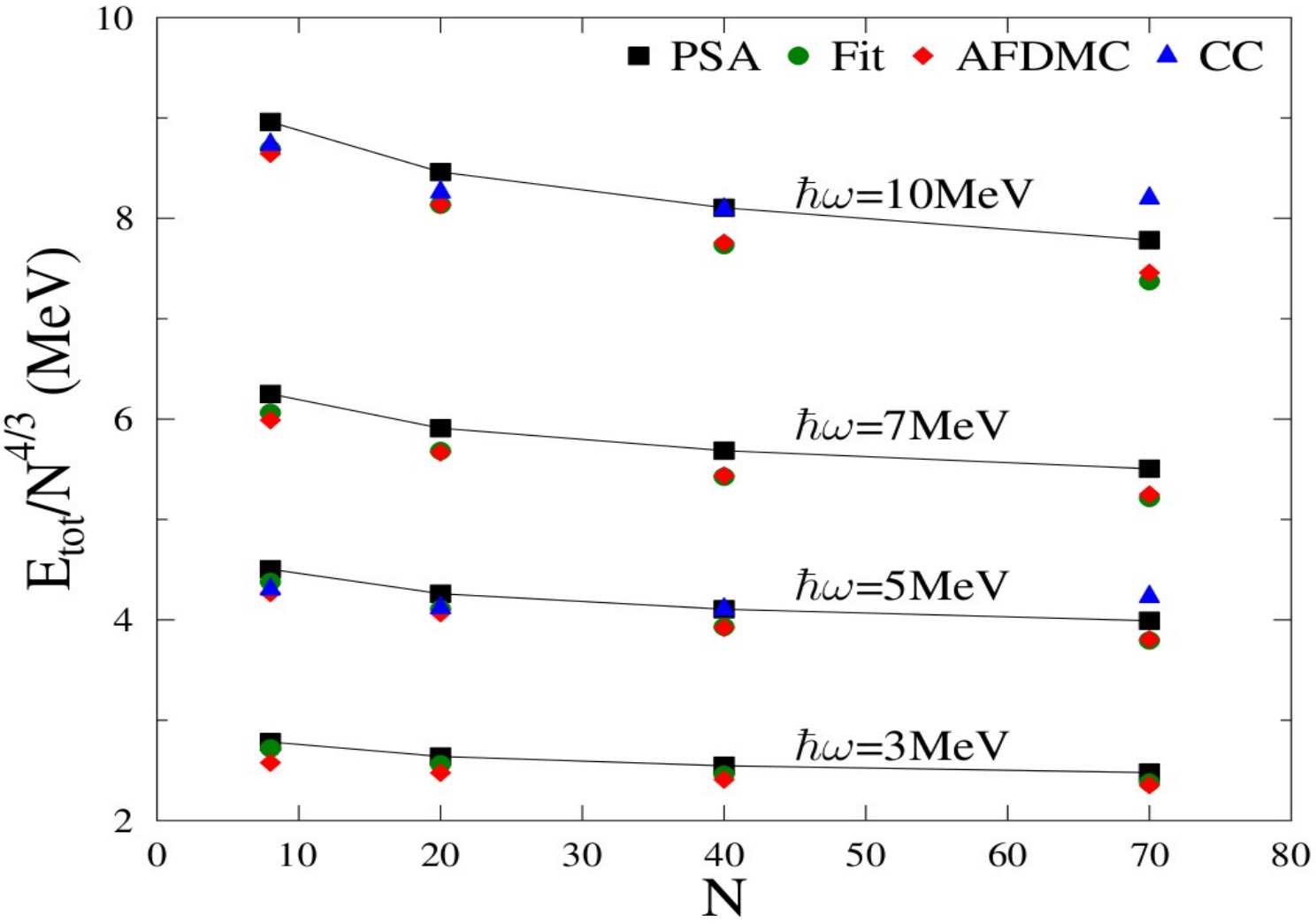
Continuation of neutron droplet study

- We plan to continue testing DME with Minnesota potential in neutron droplets
- Next step is to go to heavier droplets, include pairing, etc.
- DFT results are to be compared to AFDMC and CC results

S. Bogner, S. Gandolfi, R.J. Furnstahl, G. Hagen, H. Hergert, J. Holt, MK, M. Stoitsov, In progress

Continuation of neutron droplet study

Preliminary results



Fitted results optimized to AFDMC total energies

S. Bogner, S. Gandolfi, R.J. Furnstahl, G. Hagen, H. Hergert, J. Holt, MK, M. Stoitsov, In progress

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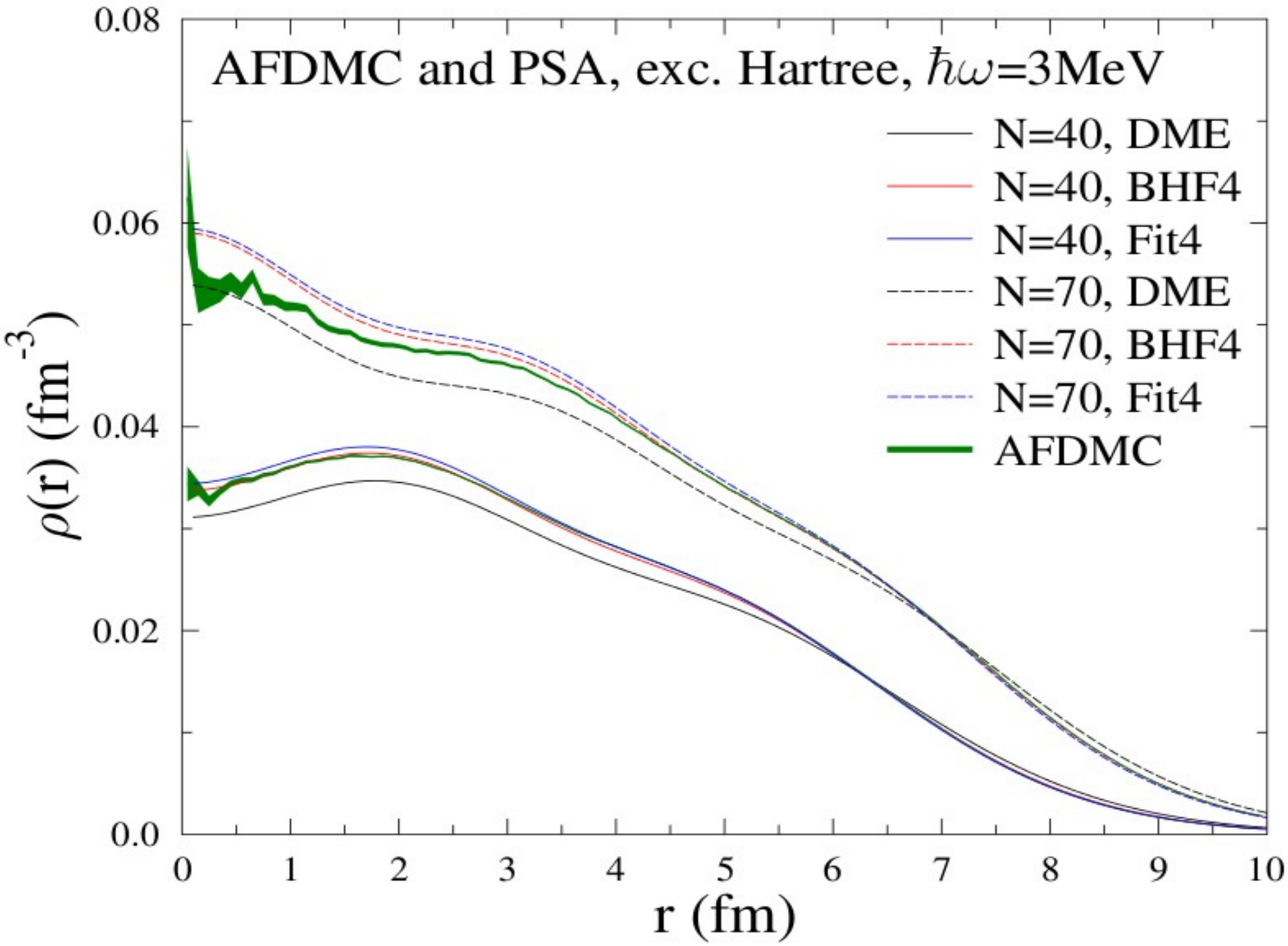

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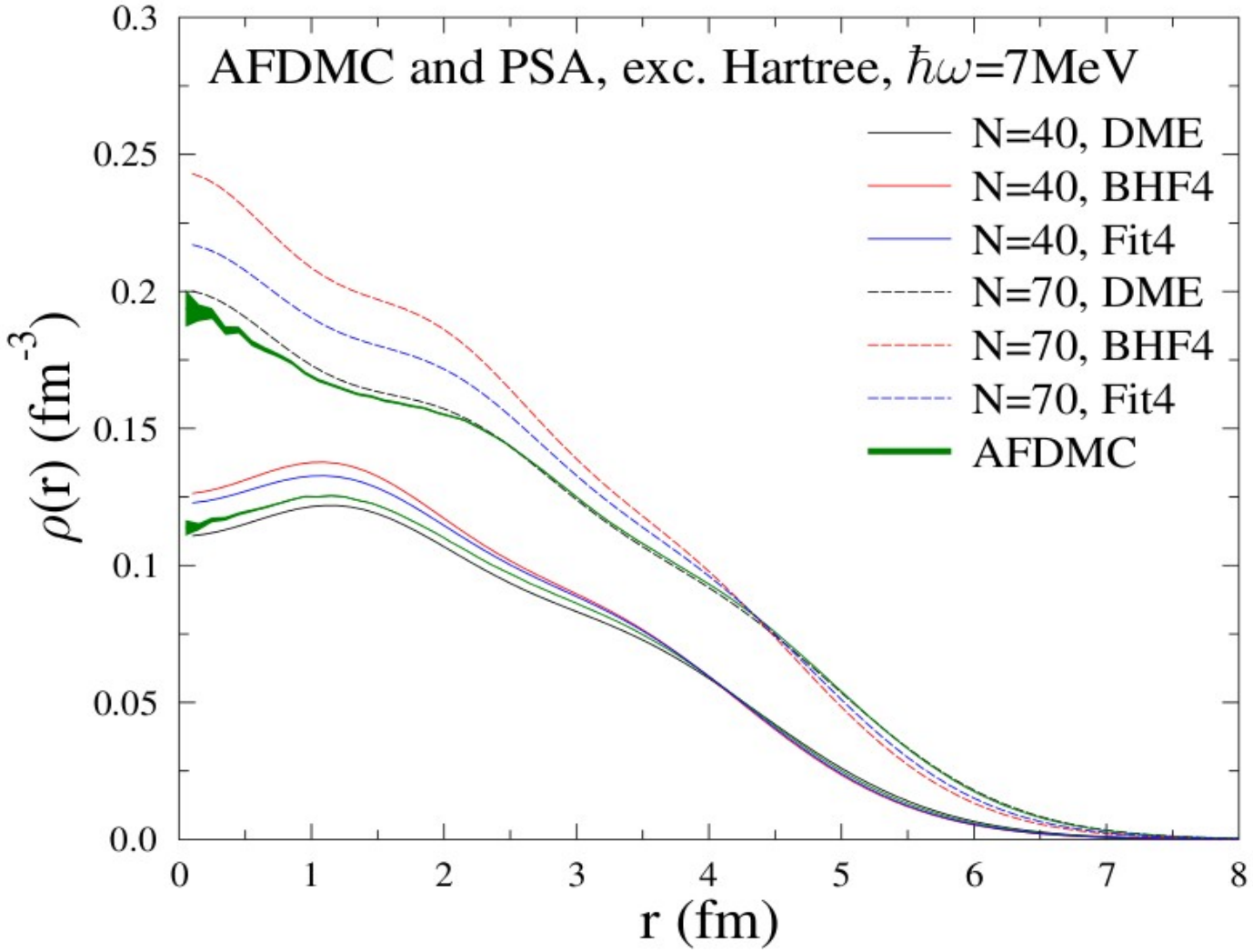
Continuation of neutron droplet study

Preliminary results



S. Bogner, S. Gandolfi, R.J. Furnstahl, G. Hagen, H. Hergert, J. Holt, MK, M. Stoitsov, In progress

Continuation of neutron droplet study

Preliminary results

- Comparison of root mean-squared deviations between Skyrme and DME functional, both fitted to the same AFDMC total energies (14 droplets):

	RMS Etot (MeV)	RMS radii (fm)
Skyrme	5.1	0.070
DME	4.3	0.062

Skyrme density dependence: $\gamma = 1/6$

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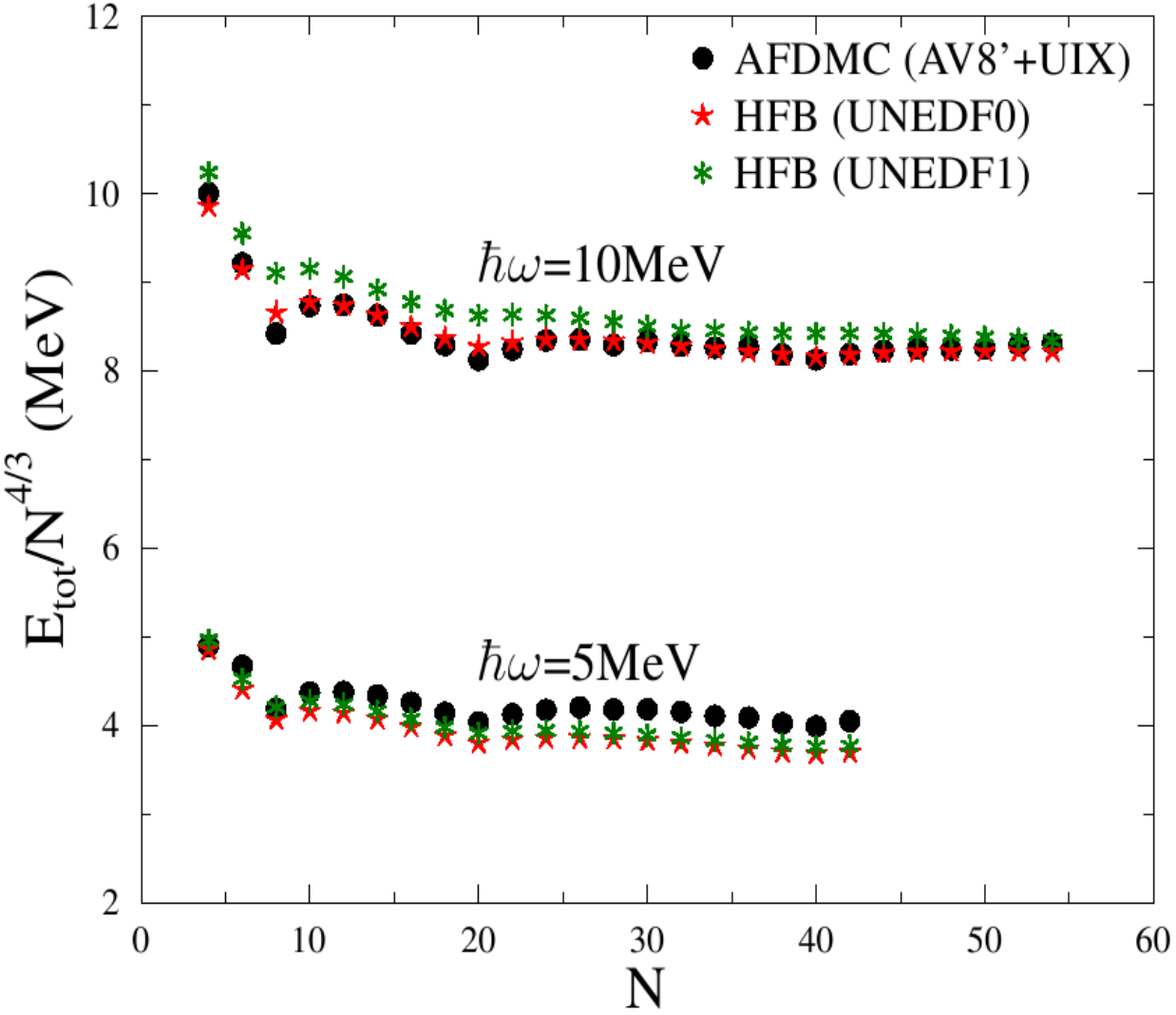
Optimizing EDF to neutron droplet data

Neutron droplets and DFT optimization

- future EDF optimization could utilize ab-initio data on neutron droplets to constrain currently poorly determined coupling constants
- droplet data constrains both, bulk and surface properties of the EDF
- improves description of very neutron rich nuclei.
- AFDMC, NCFC, and CC results could be used in the future for UNEDF3 or UNEDF4 optimization
- both, energies and radii useful for EDF optimization



AFDMC results by S. Gandolfi, J. Carlson, Steven C. Pieper, PRL 106, 012501 (2011)
UNEDF0: PRC 82, 024313 (2010)
UNEDF1: PRC 85, 024304 (2012)

Some Conclusions

- DME can be used to construct a semi-local EDF from chiral potential (or from some other potential)
- Pre-optimized χ-based EDF seems to work on the selected data set somewhat better than Skyrme
- In future χ-based EDF will be optimized with the UNEDF procedure. This can be then compared to Skyrme optimized with identical data set
- DME functional expected to work better than Skyrme
- Neutron droplets offer a tool to test DME
- DME functional with contact terms added reproduces NCFC and AFDMC results in neutron droplets well
- Ab-initio results on neutron droplets can be used as a pseudo-data on optimization of EDF