Neutron droplets in DFT

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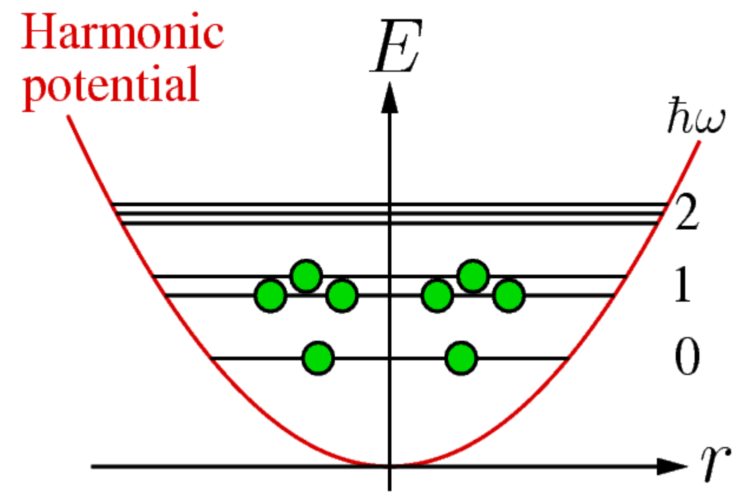
Neutron droplets and DFT

- 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

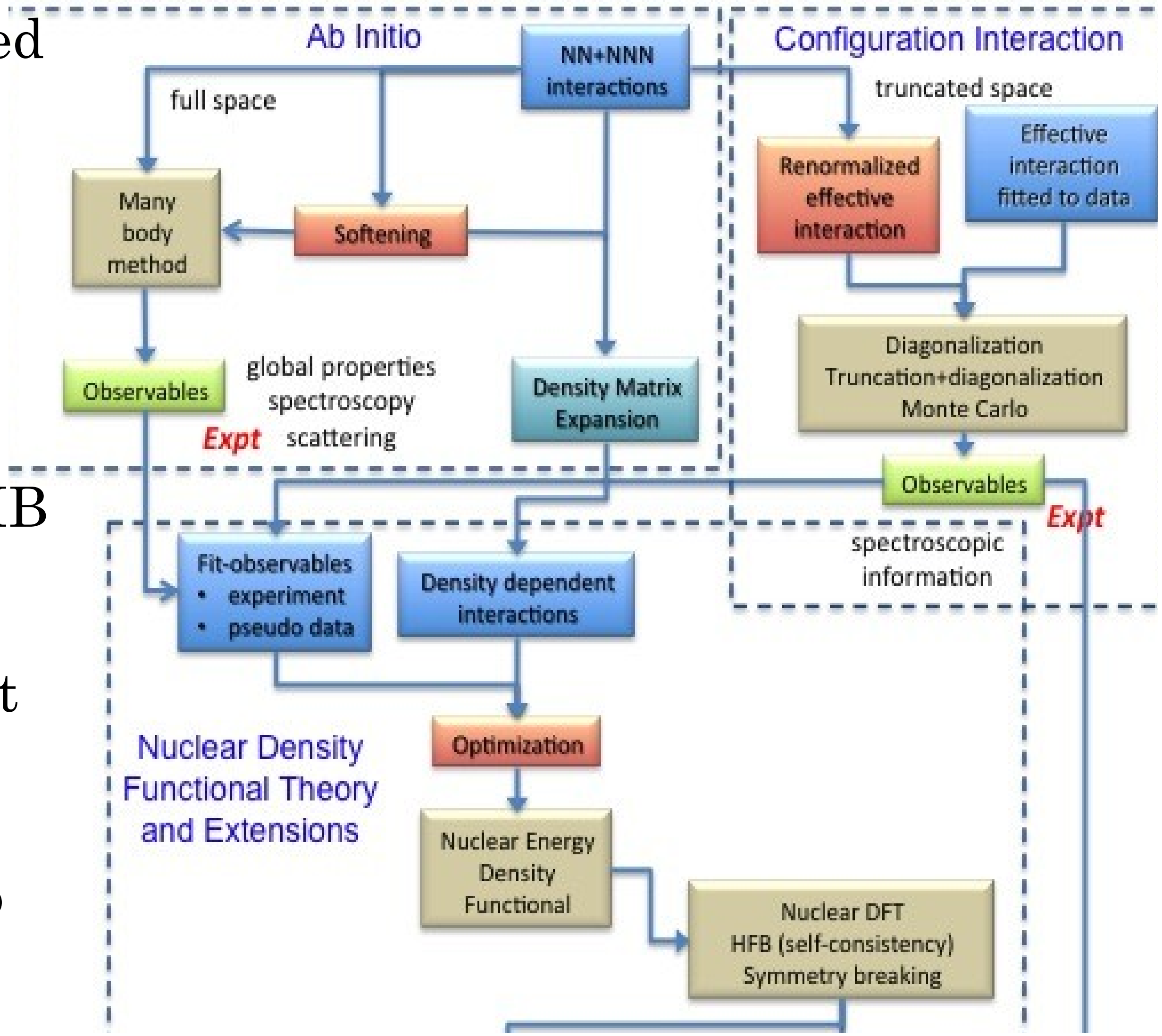


Testing the density matrix expansion against ab initio calculations of trapped neutron drops

S.K. Bogner, R.J. Furnstahl, H. Hergert,
MK, P. Maris, M. Stoitsov, and J.P. Vary,
arXiv:1106.3557 [nucl-th]

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 of the same potential
- 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

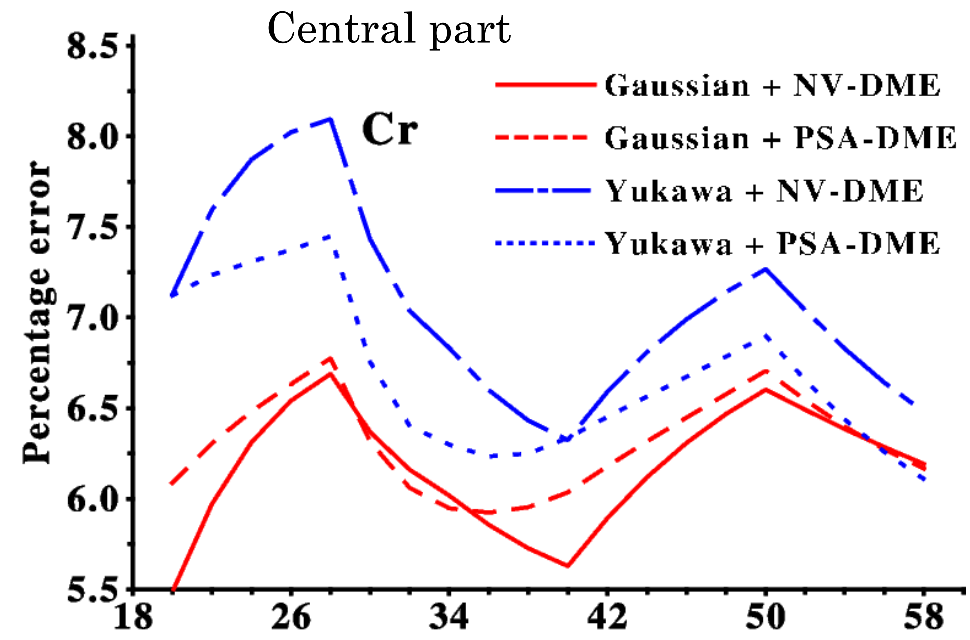


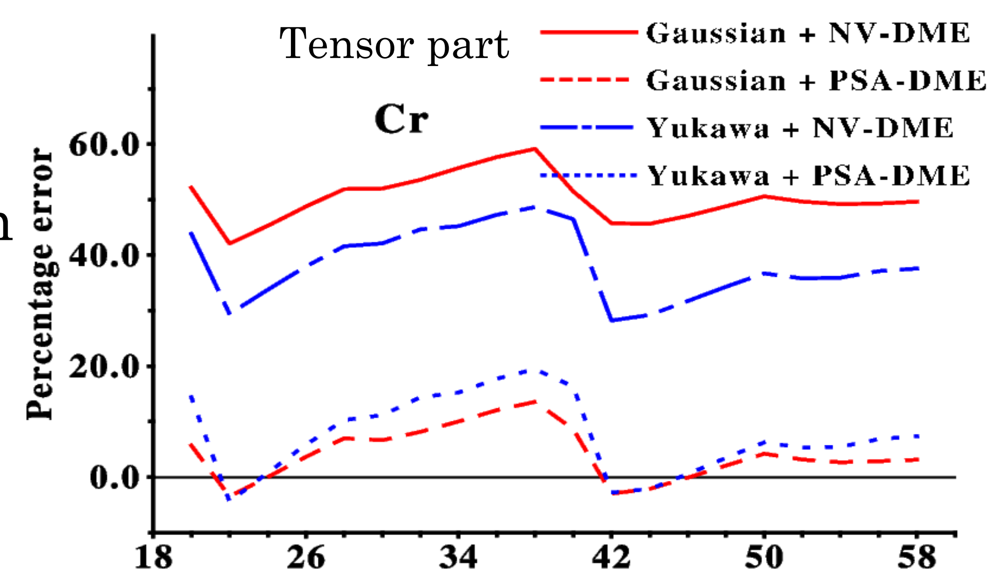
Density matrix expansion

- we have used Negele-Vautherin (NV) and phase-space averaging (PSA) DME
- 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
- for PSA see B. Gebremariam, T. Duguet, and S. K. Bogner, PRC82, 014305 (2010) and S. Bogner's talk on last year's UNEDF meeting
- DME expressions in HFB solvers handled with similar module as in χ-DME EDF case

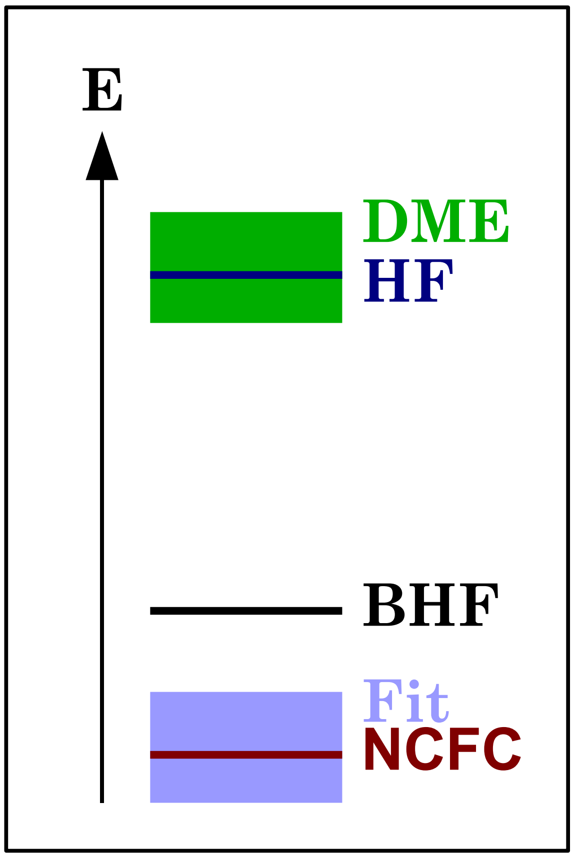




From PRC82, 014305 (2010)

Comparison of different many body methods

Expected energies



- Minnesota potential (NPA286, 53 (1977)) provides a simple and nontrivial 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. Results from this EDF can be compared exact HF calculation
- 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

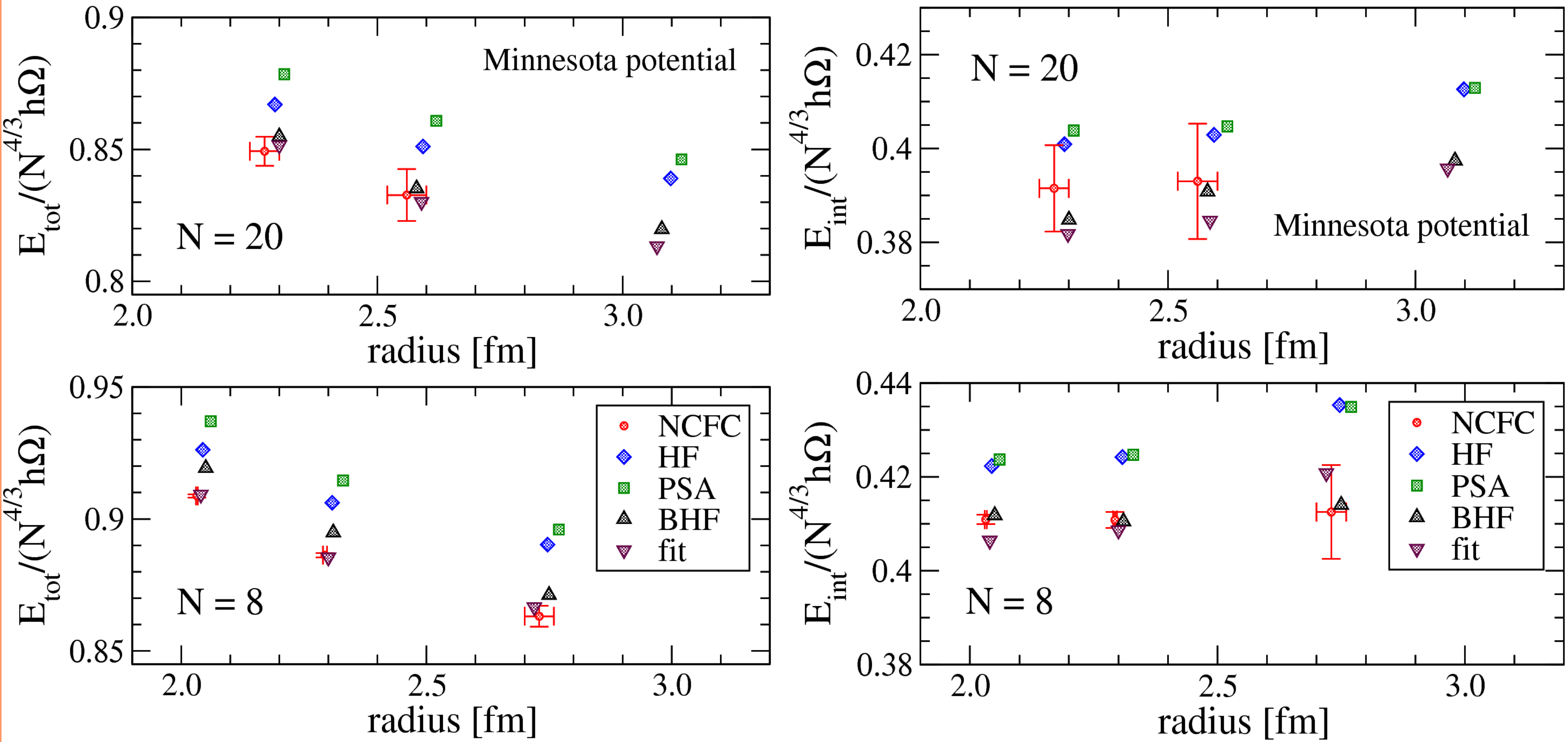
- DME can be applied to the Fock term, or on both Hartree and Fock terms
- PSA with exact treatment of Hartree term provides closest results to exact HF
- DME energies calculated from exact HF densities are almost identical to self consistent DME energies

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

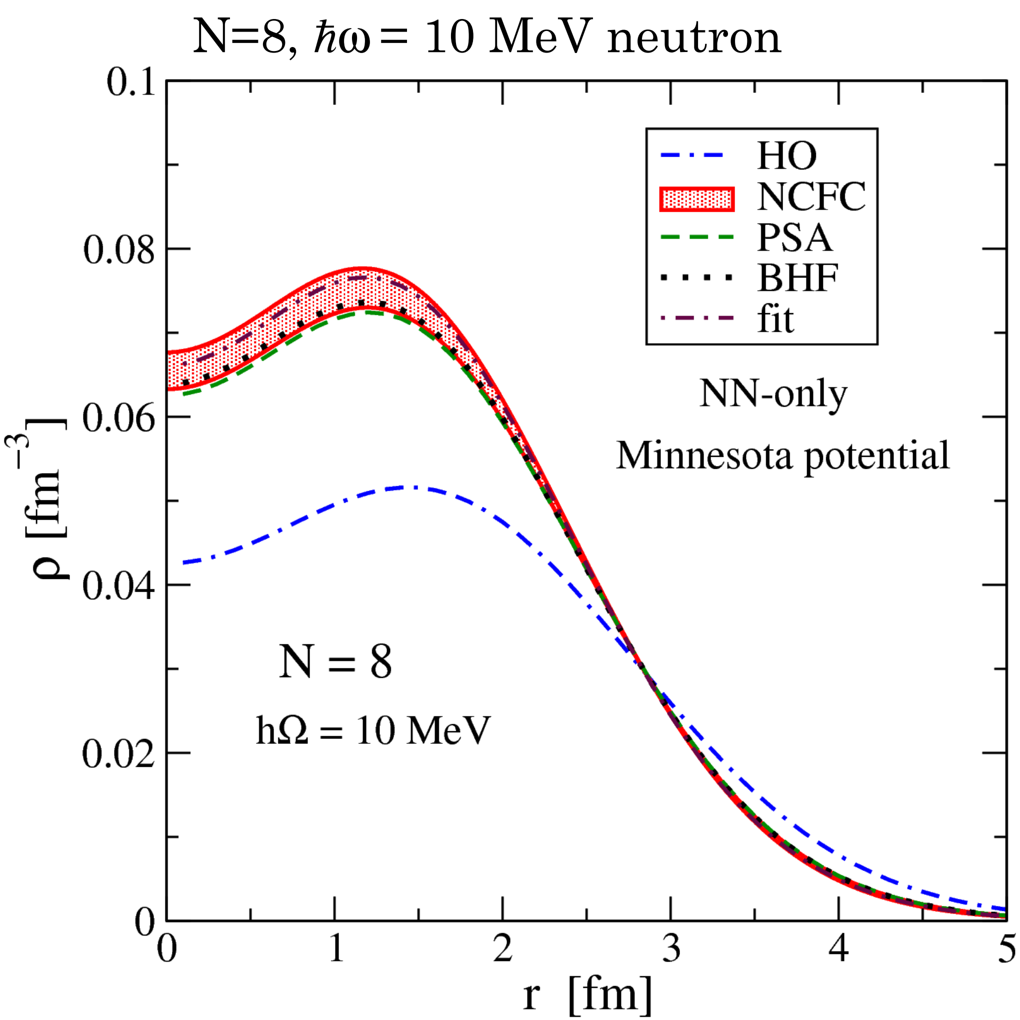
DFT and NCFC results compared

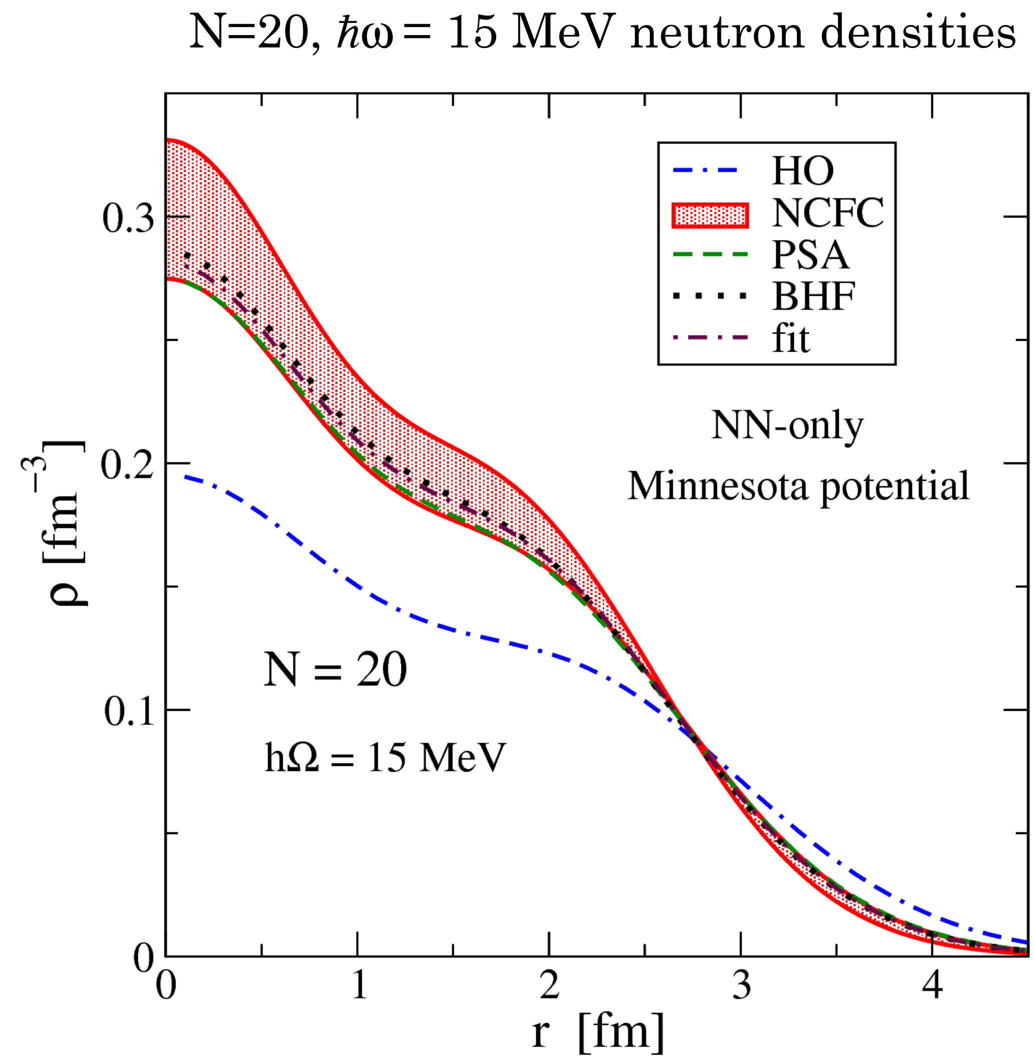
Total energies | Internal energies



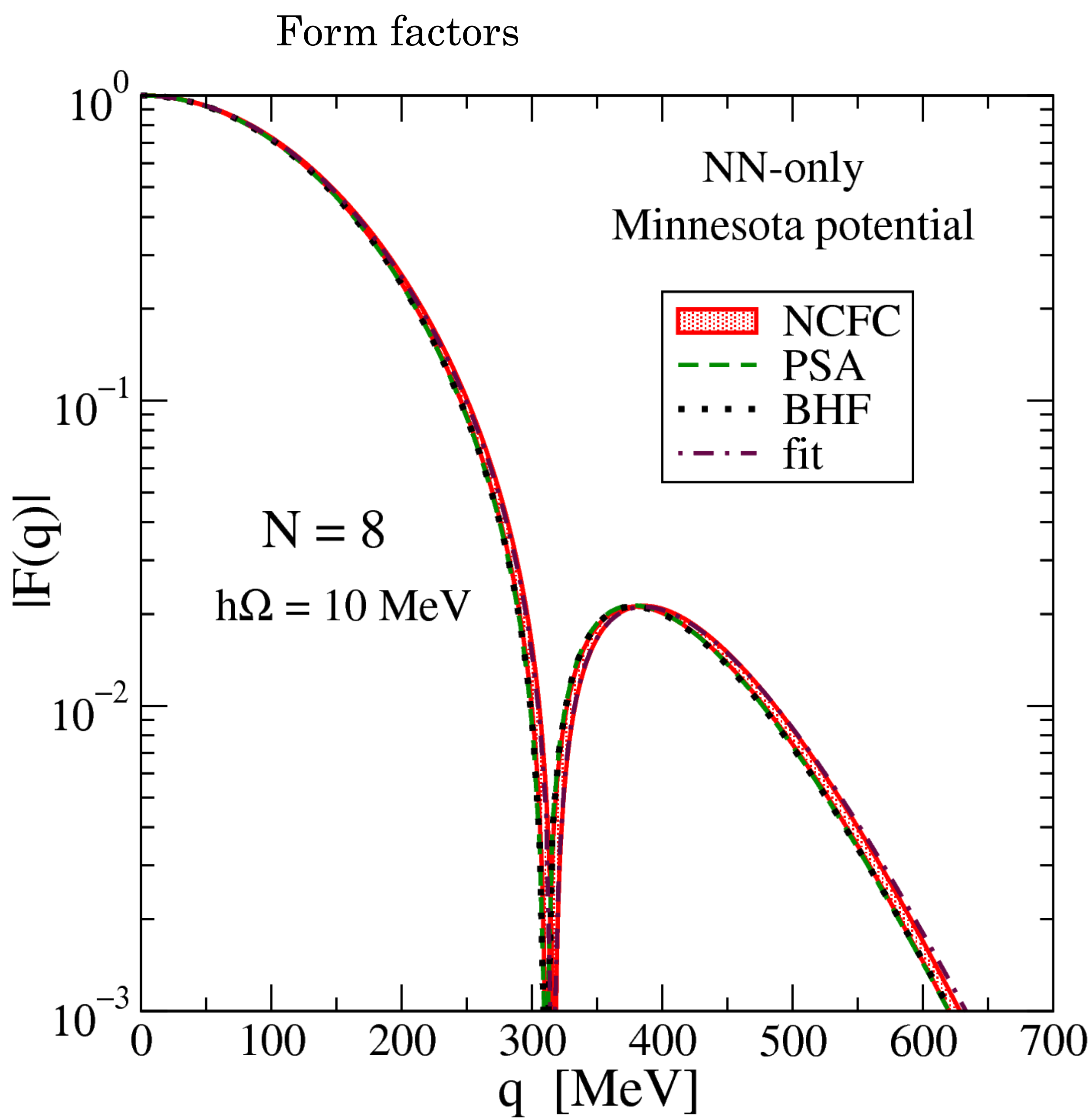
$\hbar\omega = 20, 15, 10$ MeV (from left to right in figures)

DFT and NCFC results compared





DFT and NCFC results compared



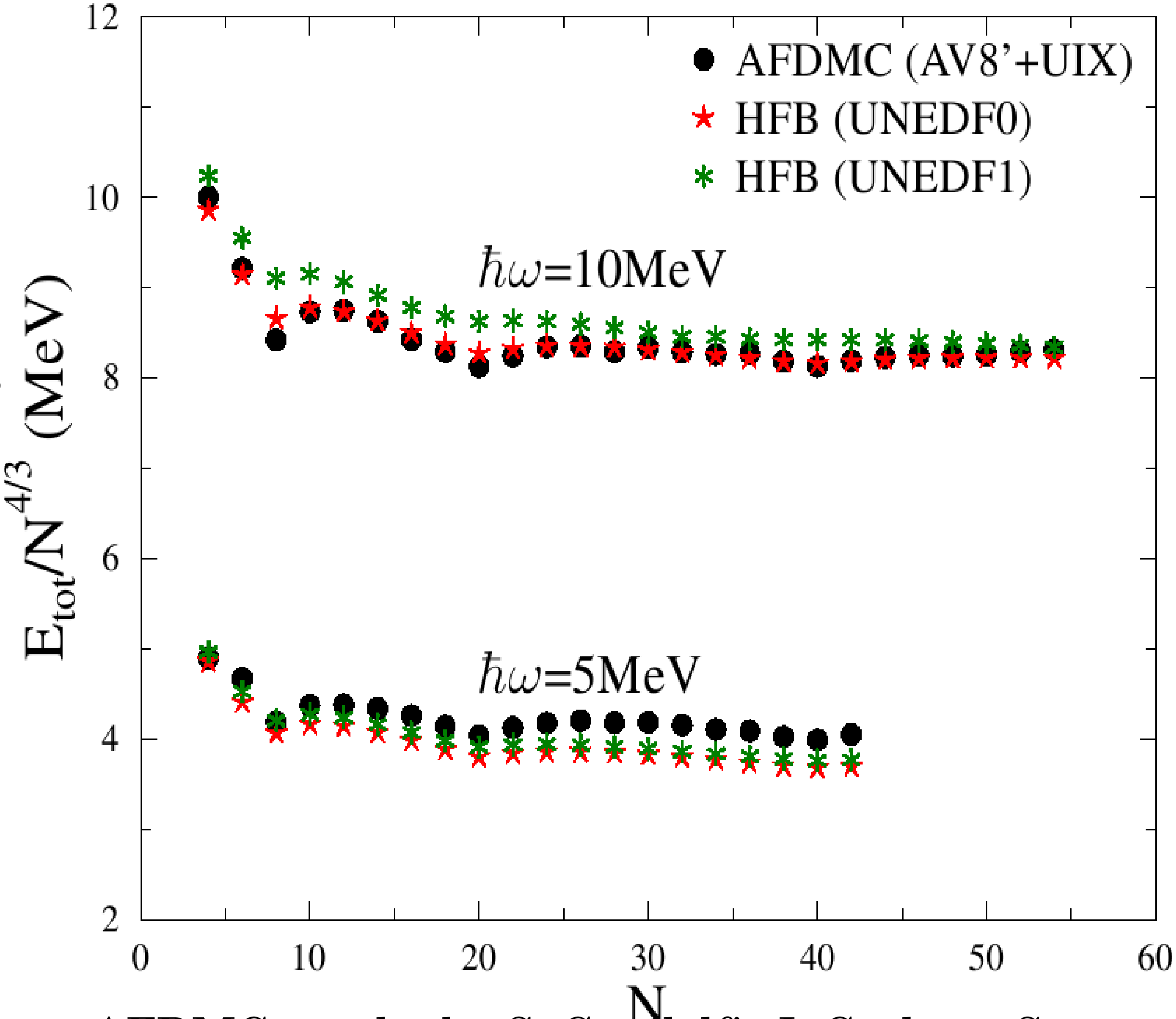
Some Conclusions

- neutron droplets provide a controllable environment to test different many-body methods
- PSA with exact treatment of Hartree term closest to exact HF results
- BHF results closer to NCFC results than bare DMA results, but still outside of the theoretical error bars
- Fit results often inside of the theoretical error bars, but not always. Generally they have good agreement
- year 5 deliverables: neutron drop calculations from NN interaction validated against ab-initio calculations
- next step: test χ-DME EDF against exact HF and ab-initio calculations, include pairing

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 and NCFC results could be used in the future for UNEDF2 or UNEDF3 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: to be published (see N. Schunck's talk)

Additional slides

Comparison of NV and PSA DME to HF

Difference in internal energy compared to exact HF in MeV

N	$\hbar\Omega$	HF/NV NV	HF/NV NT	HF/NV exact	HF/PSA PSA	HF/PSA NT	HF/PSA exact
8	3	0.0	−0.0	0.0	0.1	0.0	0.1
8	5	−0.1	−0.4	−0.1	0.2	−0.3	−0.1
8	10	0.1	−1.0	−0.2	1.3	−1.0	−0.1
8	15	1.1	−1.5	0.3	5.4	−1.8	0.1
8	20	3.2	−1.9	1.1		−2.7	0.5
20	3	−0.2	−0.4	−0.3	0.1	−0.3	−0.1
20	5	−0.3	−1.2	−0.6	1.0	−0.8	−0.2
20	10	3.3	−2.2	0.3	11.9	−2.6	0.2
20	15	16.9	−2.0	4.4		−5.4	1.4
20	20	68.3	−1.2	11.1		−8.7	3.2

Difference in radius compared to exact HF in fm

N	$\hbar\Omega$	HF/NV NV	HF/NV NT	HF/NV exact	HF/PSA PSA	HF/PSA NT	HF/PSA exact
8	3	0.01	0.02	0.00	−0.02	0.01	−0.01
8	5	0.03	0.07	0.03	−0.01	0.05	0.01
8	10	0.04	0.11	0.04	−0.06	0.09	0.02
8	15	0.03	0.14	0.04	−0.13	0.12	0.02
8	20	0.02	0.16	0.05		0.15	0.02
20	3	0.02	0.05	0.03	−0.02	0.02	0.01
20	5	0.04	0.09	0.06	−0.04	0.06	0.02
20	10	0.02	0.13	0.07	−0.18	0.09	0.02
20	15	−0.04	0.16	0.07		0.13	0.03
20	20	−0.20	0.18	0.05		0.15	0.02

Deformation

•imposing a non-zero deformation increases total energy.