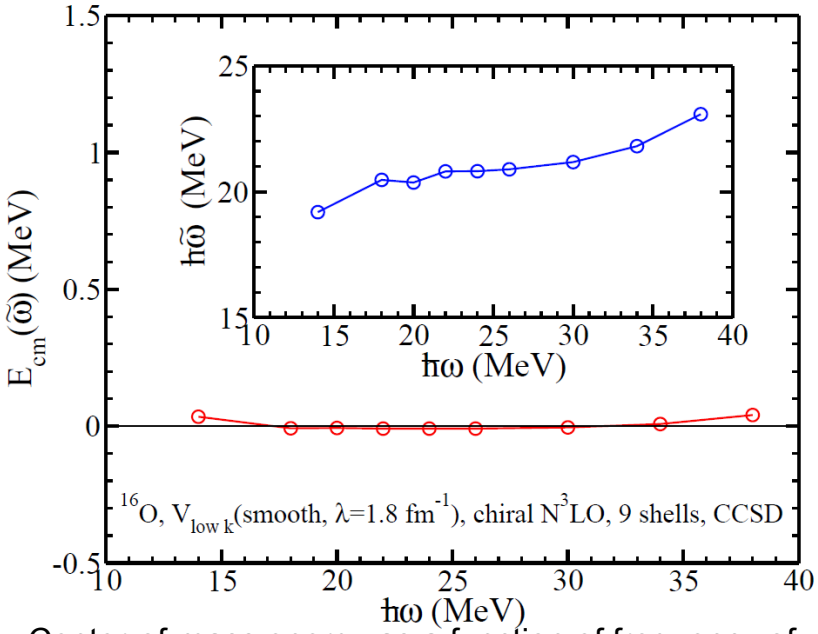
UNEDF ab-initio progress and Plans for Year 4 & 5

- Achievements/Deliverables
  - Nuclei (^{40}Ca, ^{12}C, ...)
  - Neutron Drops and Density Functionals
  - Nuclear Scattering
  - Response
- Year 3/4 plans
- Year 5 and Major Science Challenges

Highlights / Accomplishments: CC / 40Ca

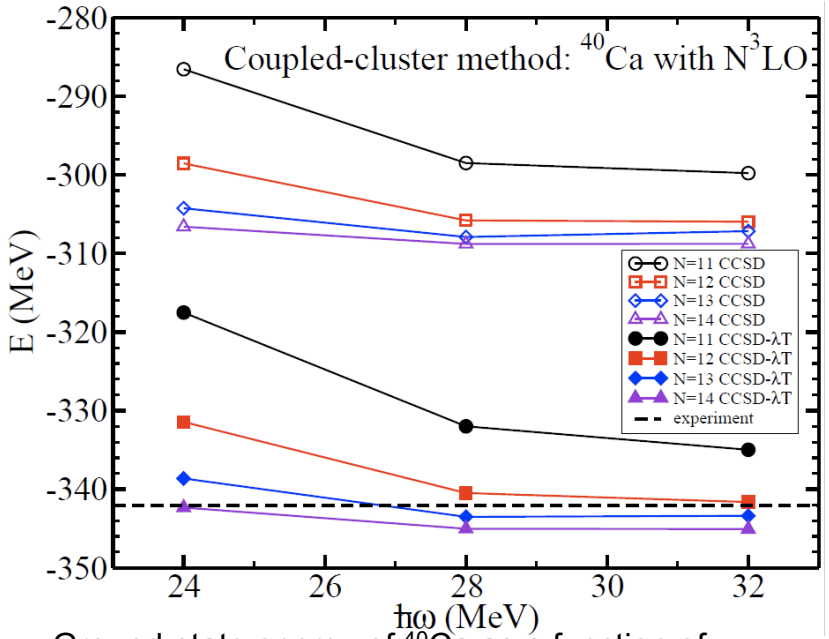
Solution of the center-of-mass problem: Coupled-cluster wave function factorizes into Gaussian center-of-mass wave function and intrinsic state. [Hagen, Papenbrock, Dean, arXiv: 0905.3167]

$$H_{\rm cm}(\tilde{\omega}) = T_{\rm cm} + \frac{1}{2}mA\tilde{\omega}^2 R_{\rm cm}^2 - \frac{3}{2}\hbar\tilde{\omega}$$



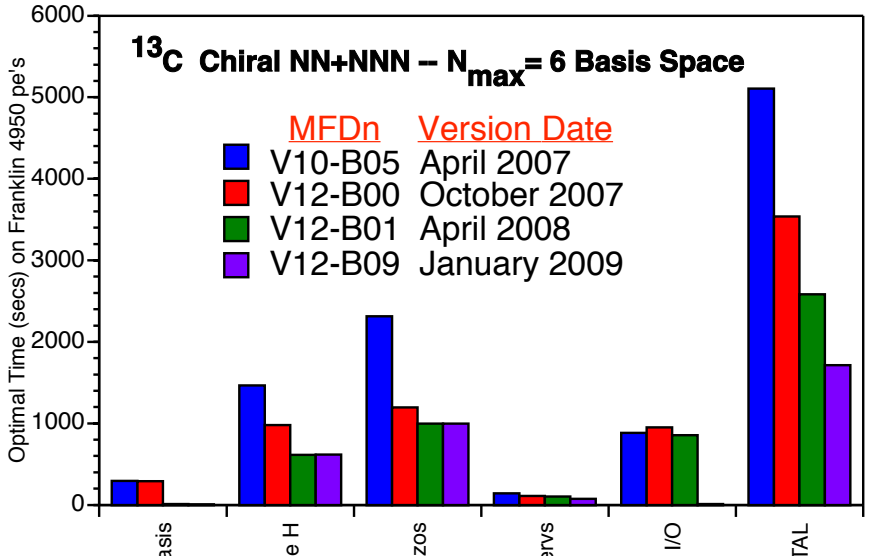
Center-of-mass energy as a function of frequency of employed oscillator basis. Inset: frequency of Gaussian center-of-mass wave function.

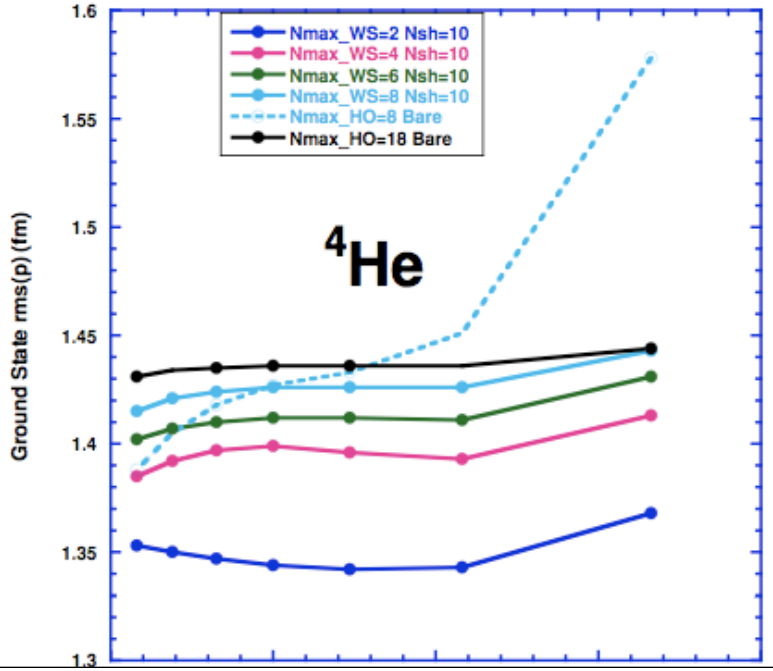
Saturation properties of chiral interactions: ^{40}Ca from a chiral nucleon-nucleon interaction within CCSD with L-triples corrections. Precision is at 2% level. [Hagen, Papenbrock, Dean, Hjorth-Jensen, Phys. Rev. Lett. 101, 092502 (2008); *ibid,* to be submitted]



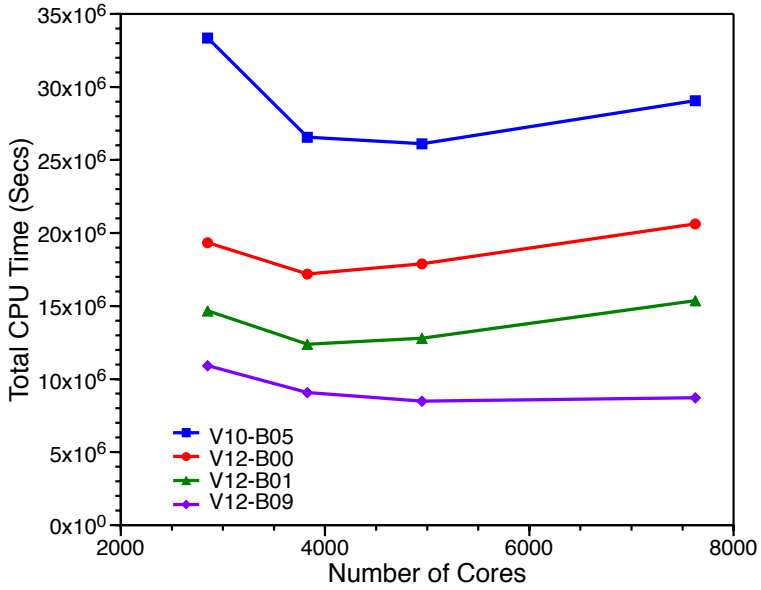
Ground-state energy of ^{40}Ca as a function of frequency of employed oscillator basis for increasing size of model space. Upper set of lines: CCSD; lower set: triples corrections.

Highlights / Accomplishments: MFDN/CI





Strong Scaling

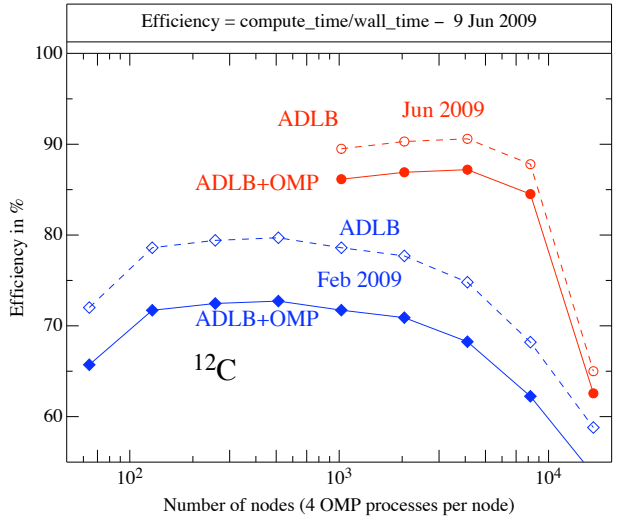


Optimized Basis

Highlights / Accomplishments: 12C / ADLB

RESULTS SO FAR

ADLB performance is very good up to 8192 nodes (32,768 cores)



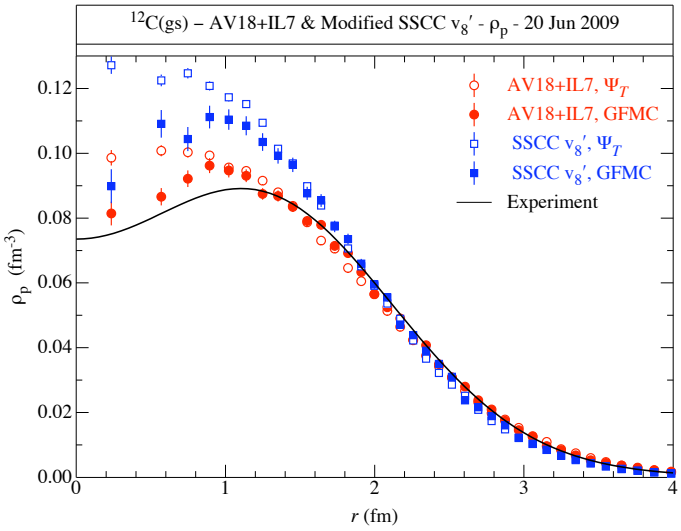
Energy

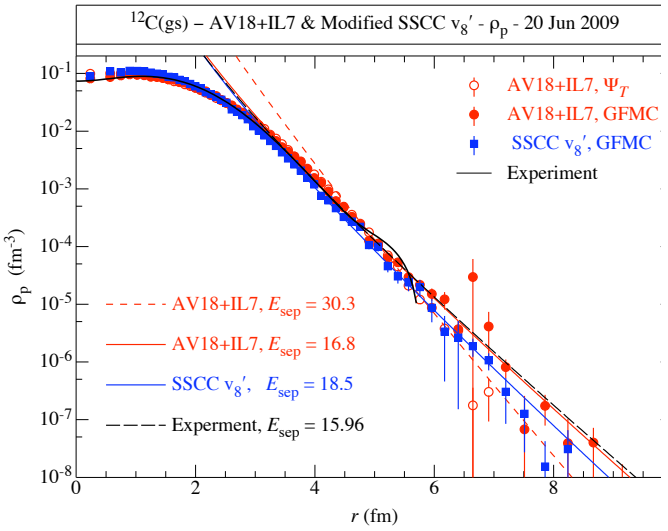
	Energy			RMS radius		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18+IL7	–65.8(2)	–93.2(6)	–92.16	2.36	2.35	2.33
Modified SSCC v_8'	–74.9(2)	–94.0(5)		2.21	2.24	

Modified SSCC v_8' gives reasonable energies at least up to $A = 12$

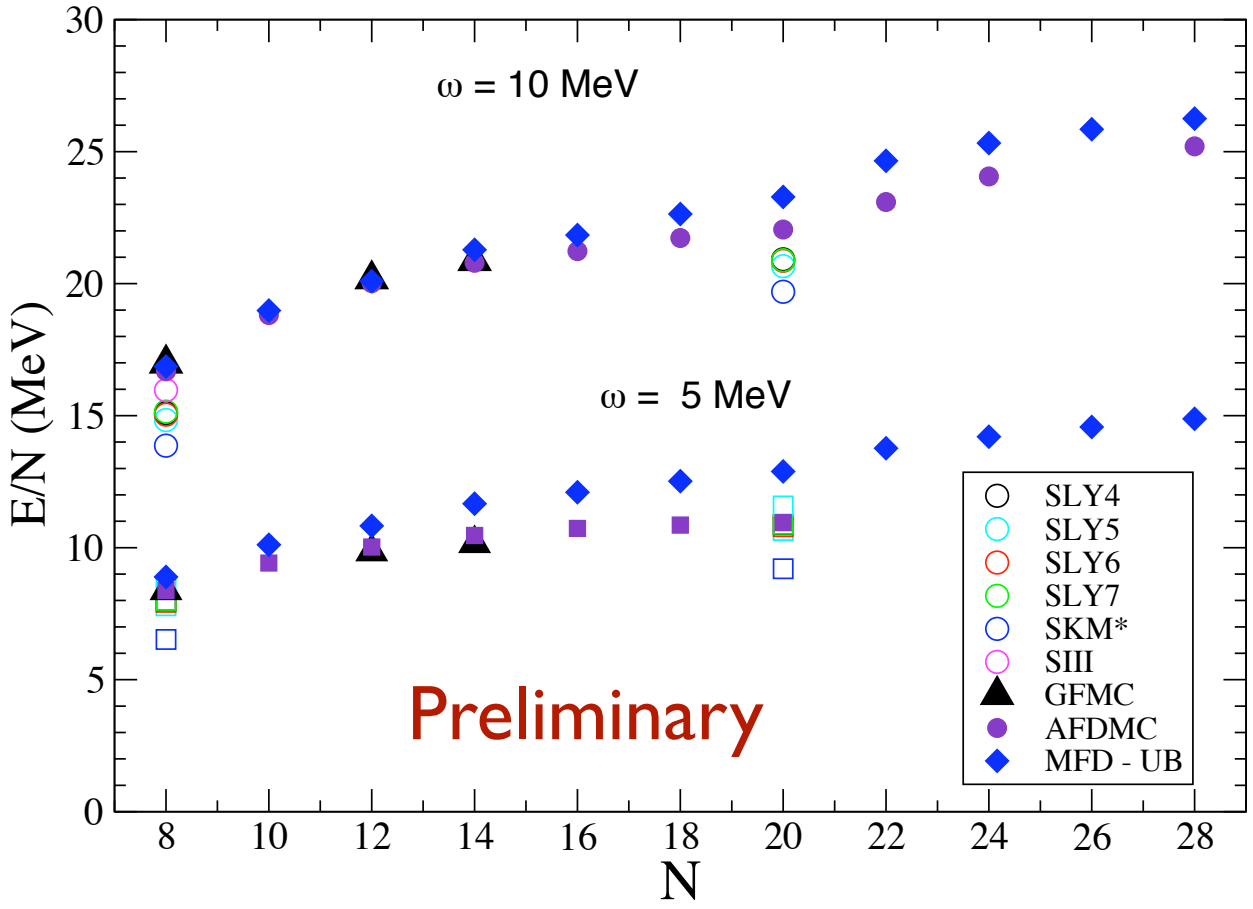
Remember that it does not accurately reproduce NN P-phase shifts

Distributions

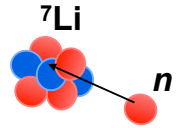




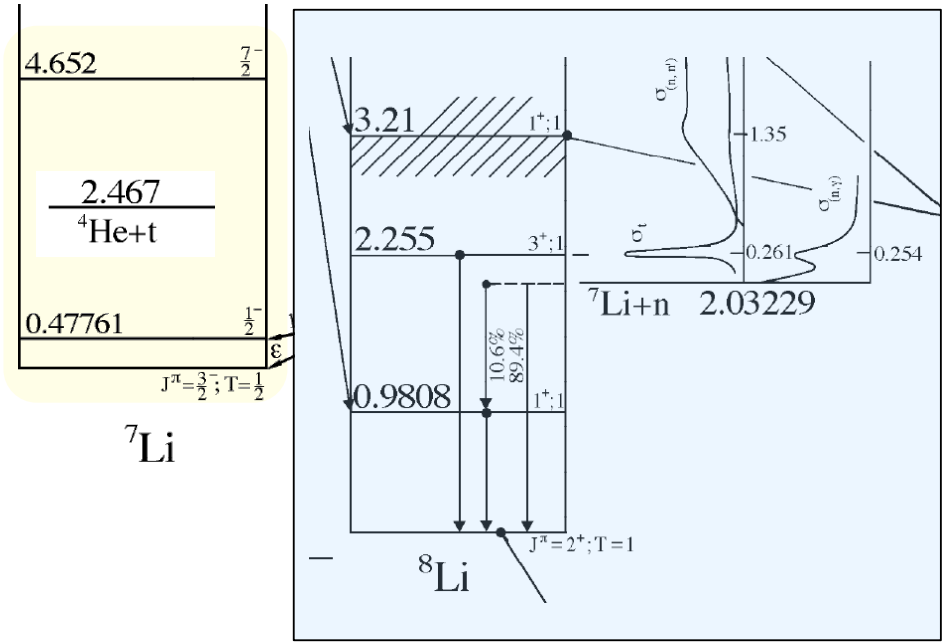
Highlights / Accomplishments: Neutron Drops

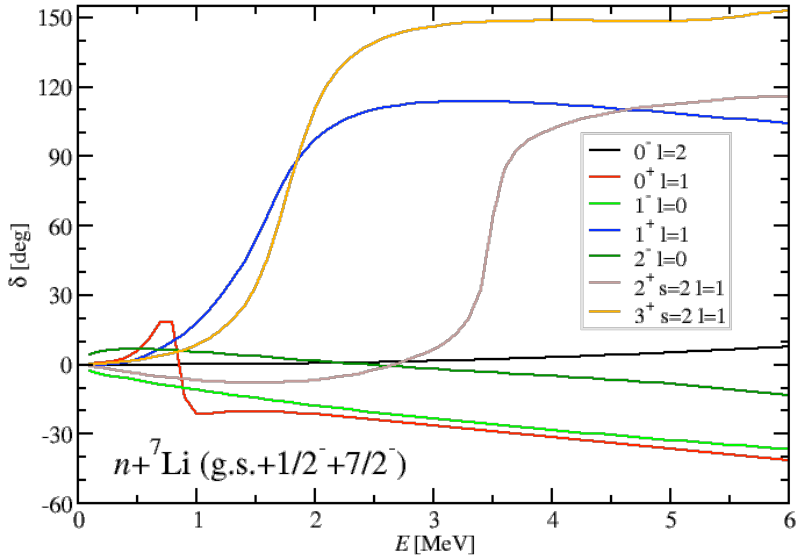


Highlights / Accomplishments: n 7Li scattering



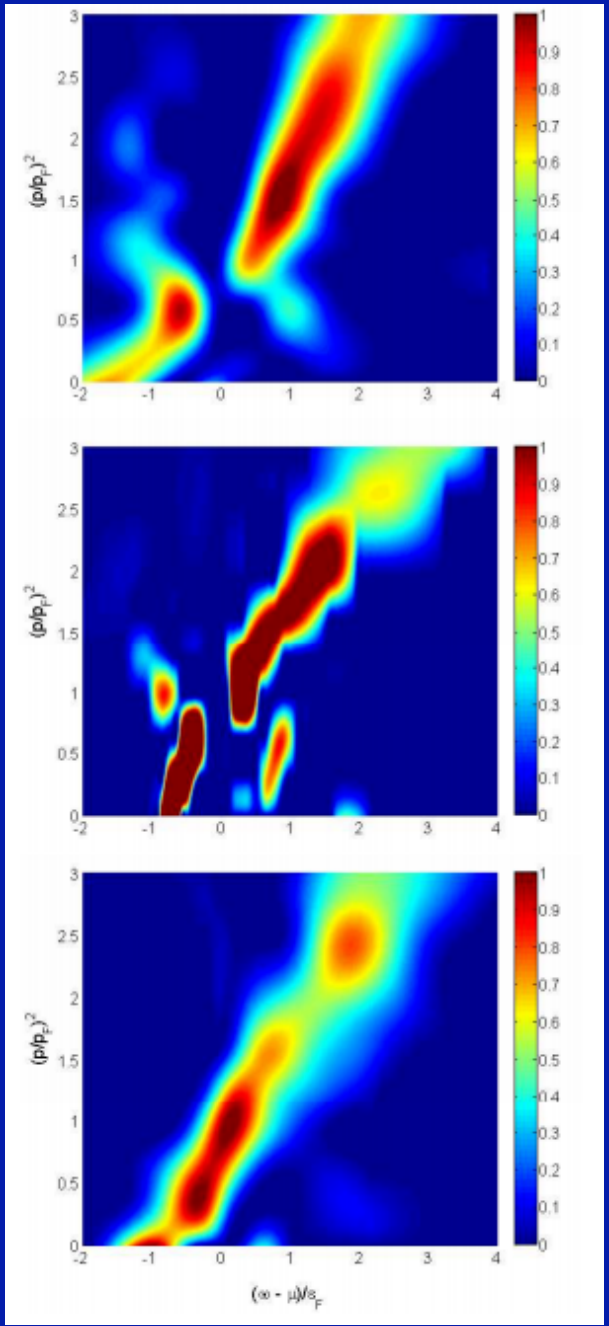
- ^{7}Li 3/2$^-$, 1/2$^-$ **and 7/2$^-$** states included
- Result for N_{max}=8 shown
- 2$^+$ and 1$^+$ states bound (slightly more)
- 0$^+$ and 1$^+$ resonances not affected
- 3$^+$ and 2$^+$ resonances appear
- Improvement of *S*-wave scattering length

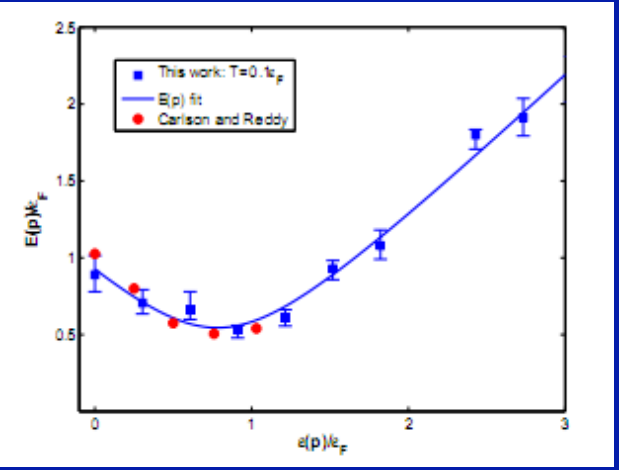


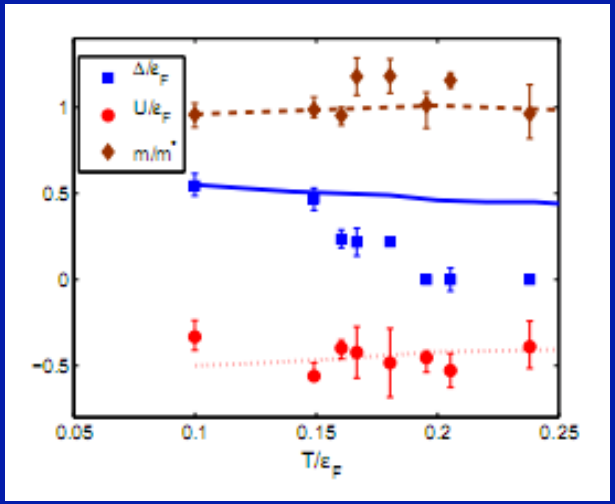


S-wave scattering length
Expt: a_{01}=0.87(7) fm
a_{02}=-3.63(5) fm
Calc: a_{01}=0.73 fm
a_{02}=-1.42 fm

Good match of bound states and narrow resonances with the ^{8}Li NCSM result.
Predicted narrow 0$^+$ and 2$^+$ resonance. Seen at recent p+^{7}Be FSU experiment.







The *ab initio* calculation of the spectral weight function, quasi-particle spectrum and its properties at finite T's.

P. Magierski, G. Wlazlowski, A. Bulgac and J.E. Drut

UNEDF ab-initio plans for year 4 (looking toward year 5)

- Nuclei
  - ^{12}C 2+ excited state and transition form factor
  - improvements to ADLB for largest computers
  - initial work toward Hoyle State
  - CI: investigation of improved basis states and conversion
  - toward ^{14}C beta decay

- Neutron Drops, External Fields, and connections to DF
  - Finish Drops including deformation, pairing, ...
  - CC interface w/ DFT
  - initial work toward ^{40}Ca DME comparisons

- Scattering
  - n-^{7}Li scattering comparisons
  - benchmarks with A=4, coupled channels in MC
  - working toward composite target, probe

High-Impact Science by Year 5

- Hoyle State in ^{12}C
- Beta Decay in ^{14}C
- DF systematic constraints from
  - neutrons
  - ^{40}Ca (CC)
  - rich external potentials, pairing, spin-orbit,...
- A=7 fusion reaction $^{3}He(\alpha,\gamma)^{7}Be$