Advances in computing nucleonic matter and nuclei from coupled-cluster theory

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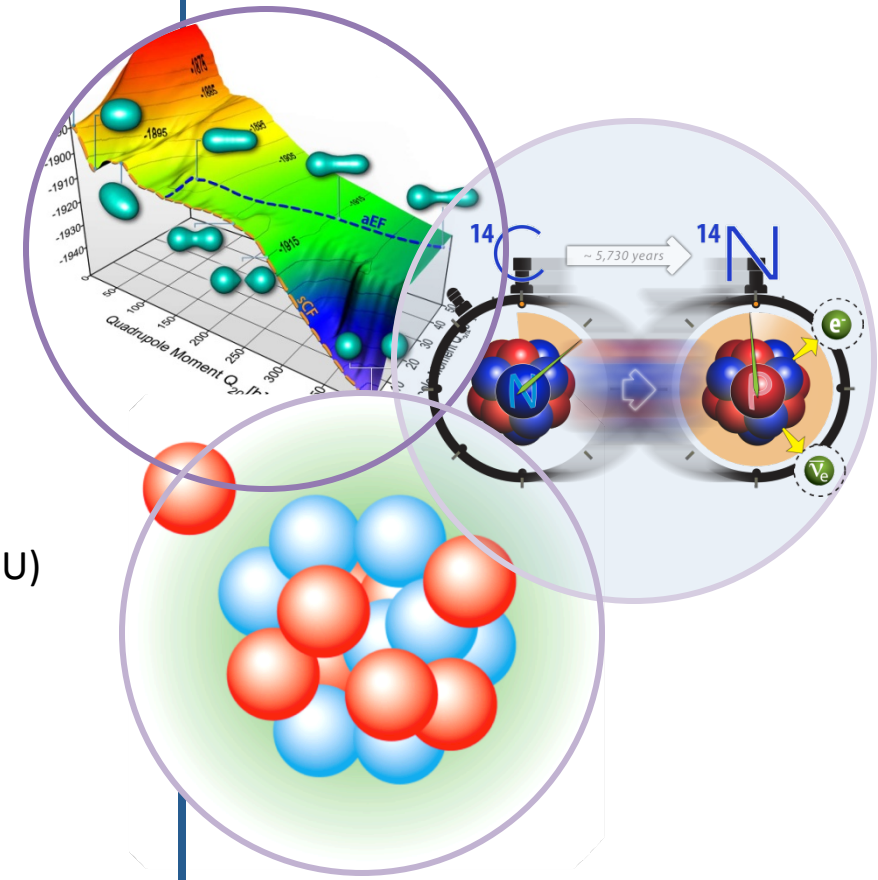

Workshop on Nuclear Structure & Reactions
TRIUMF February 9, 2014

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

arXiv:1312.7872v1 [nucl-th] 30 Dec 2013

Coupled-cluster computations of atomic nuclei

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Abstract. In the past decade, coupled-cluster theory has seen a renaissance in nuclear physics, with computations of neutron-rich and medium-mass nuclei. The method is efficient for nuclei with product-state references, and it describes many aspects of weakly bound and unbound nuclei. This report reviews the technical and conceptual developments of this method in nuclear physics, and the results of coupled-cluster calculations for nucleonic matter, and for exotic isotopes of helium, oxygen, calcium, and some of their neighbors.

PACS numbers: 21.10.Dr, 21.60.-n, 31.15.Dv, 21.30.-x

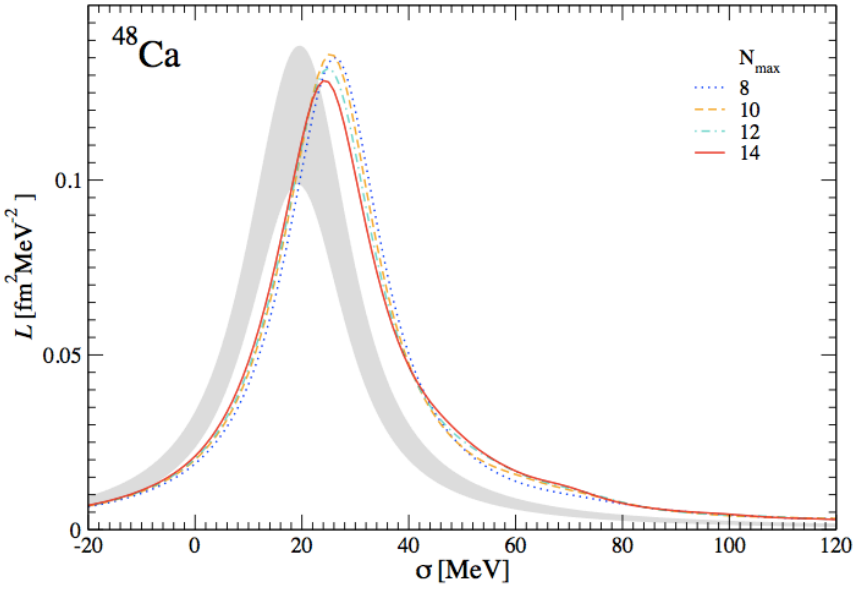
arXiv:1312.7872 (2013)

Outline

1. Elastic scattering on medium mass nuclei from coupled-cluster theory
   - Description of elastic proton scattering on ^{40}Ca
   - Halo EFT with input from ab-initio coupled-cluster calculations – Efimov physics around ^{60}Ca
2. Coupled-cluster computations of nucleonic matter with chiral NN and 3N interactions.
   - Role of particle-hole correlations in nuclear matter
   - Regulator dependence of chiral 3NFs - local or non-local?

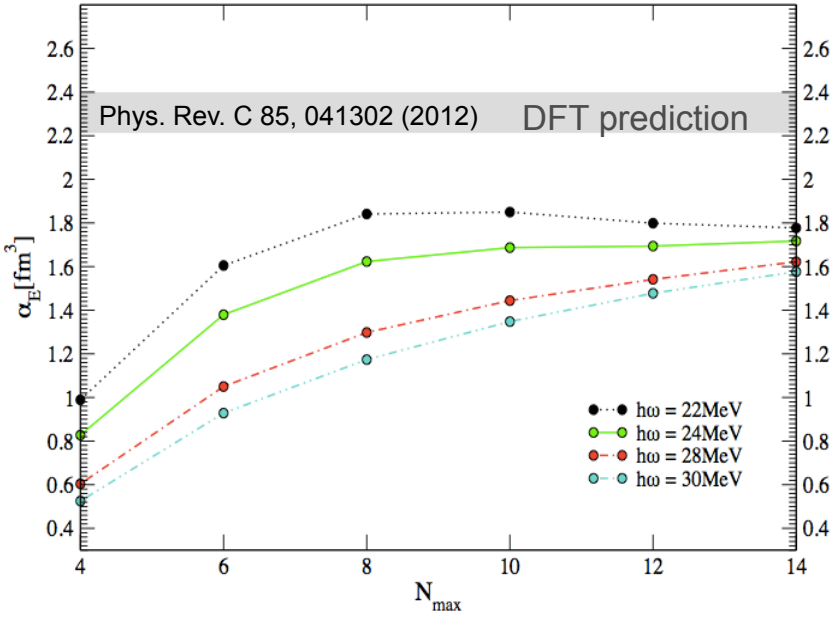
Electromagnetic reactions in medium mass nuclei

See M. Miorelli's (TRIUMF/Trento) talk on Thursday.



S. Bacca *et al*, PRL **111**, 122502 (2013)

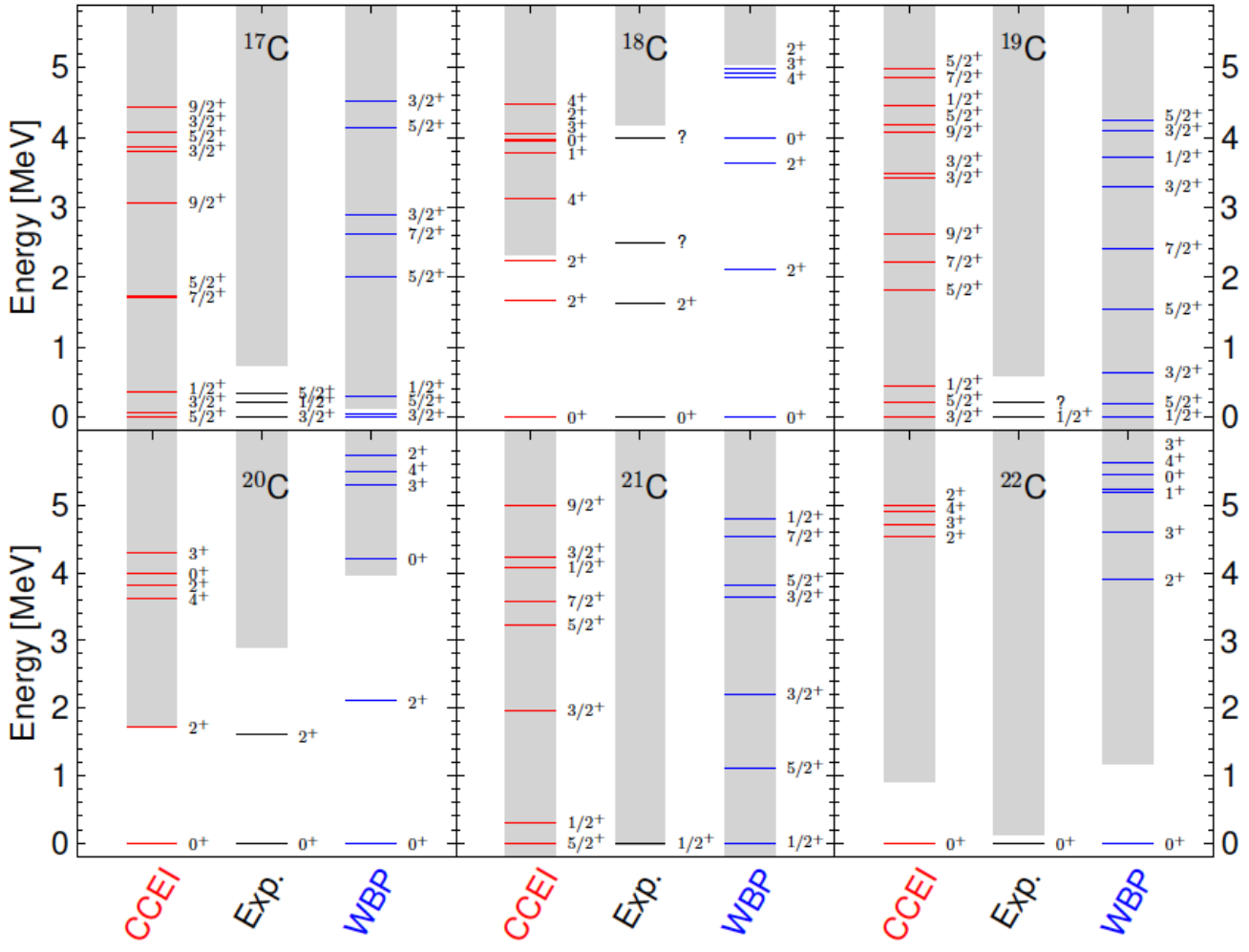
Electric Dipole Polarizability in ^{48}Ca



Coupled-cluster effective interactions for the shell-model

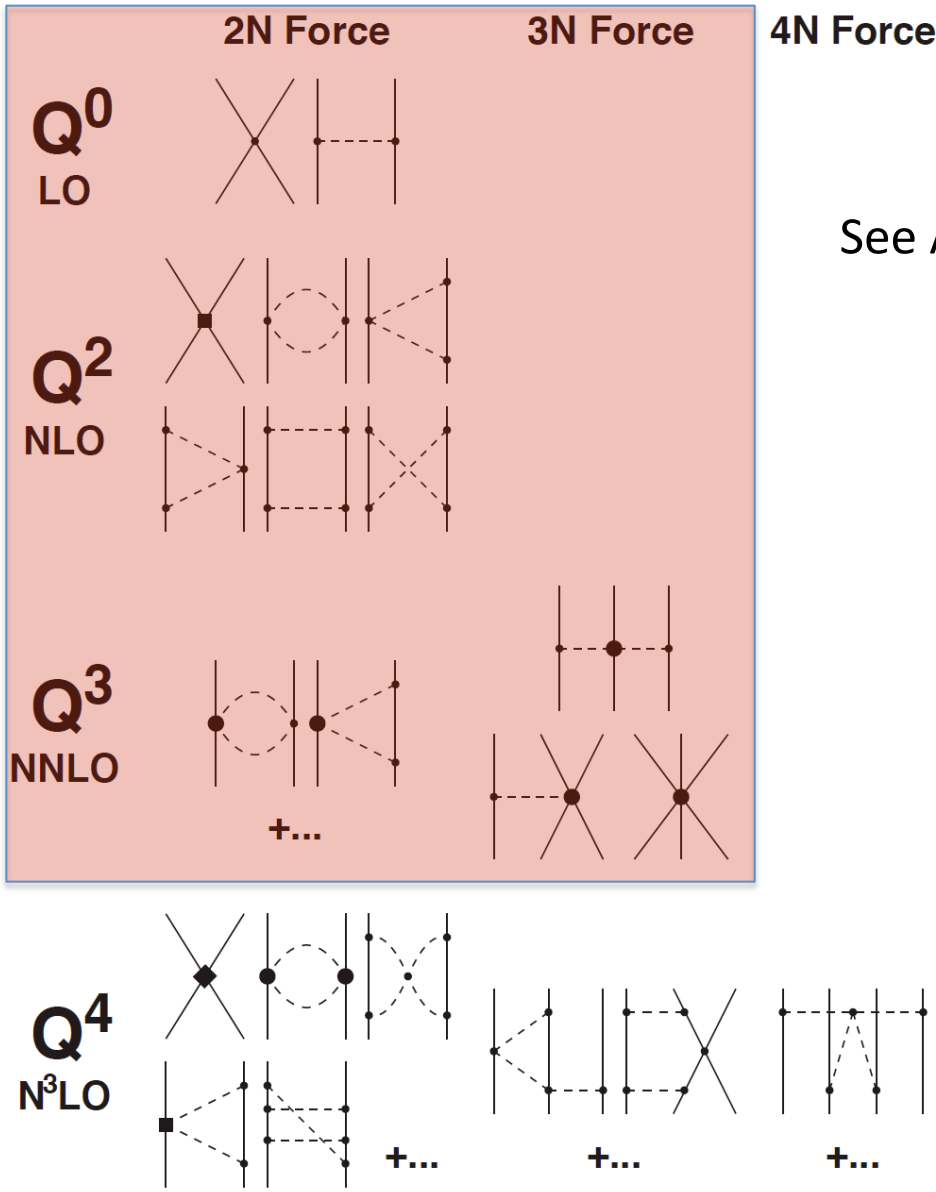
See G. Jansen's (UTK/ORNL) talk on Friday.

G. Jansen *et al* arXiv:1402.2563 (2014)



Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al.*; Entem & Machleidt; …]



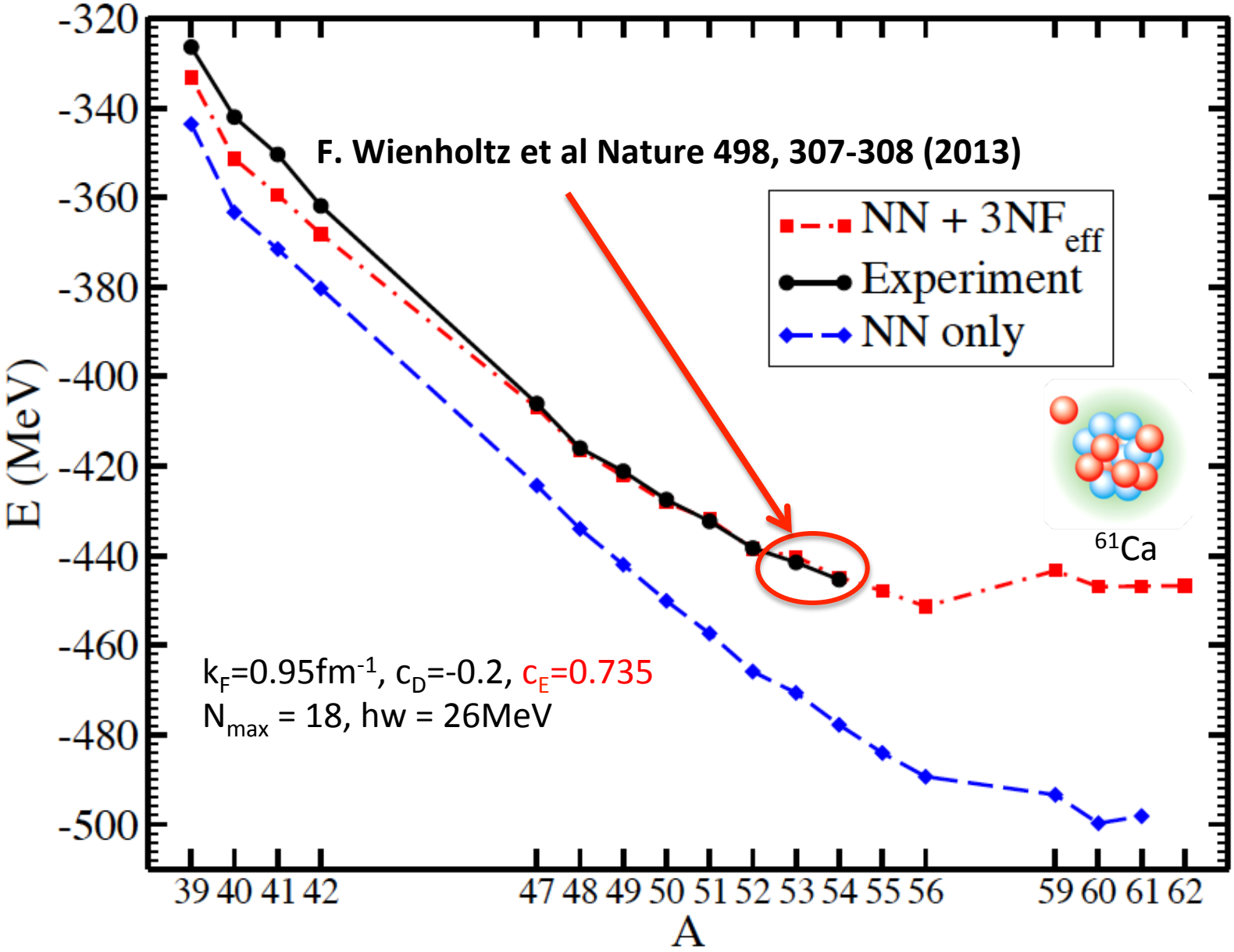
See A. Ekstrom's (UiO/Chalmers) talk on Friday.

Chiral Hamiltonian for practical use:

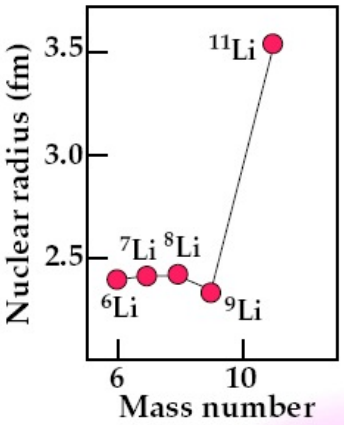
- Order-by-order: optimization of the parameters order-by-order
- Optimization strategy: Fit LEC's that enter NN and 3N sector simultaneously to observables in light and medium mass nuclei.
- Parameter uncertainties: Covariance and sensitivity analysis of parameters in few- AND many-body systems

Calcium isotopes from chiral interactions

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).



Physics of nuclei at the edges of stability



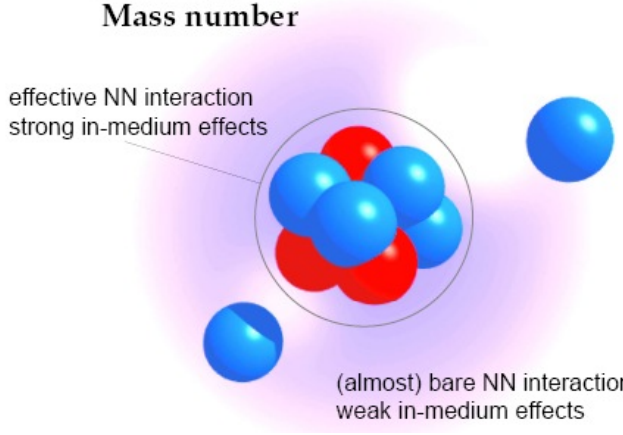
I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

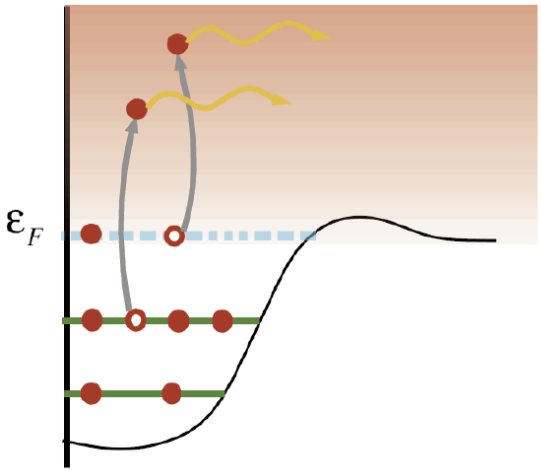
Interaction cross section measurements at Bevalac (790 MeV/u)

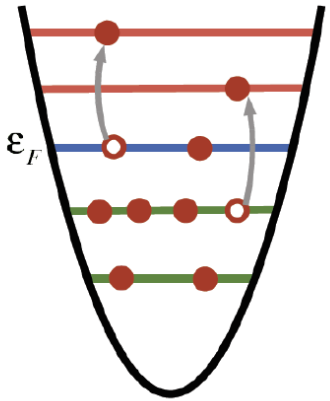
The Berggren completeness treats bound, resonant and scattering states on equal footing.

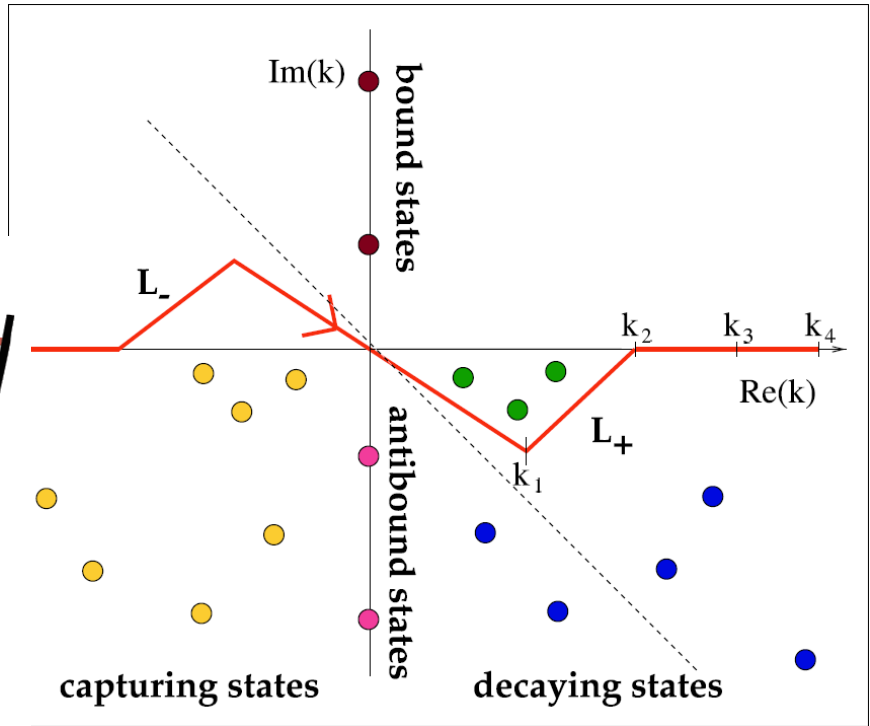
Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).









Elastic proton/neutron scattering on 40Ca

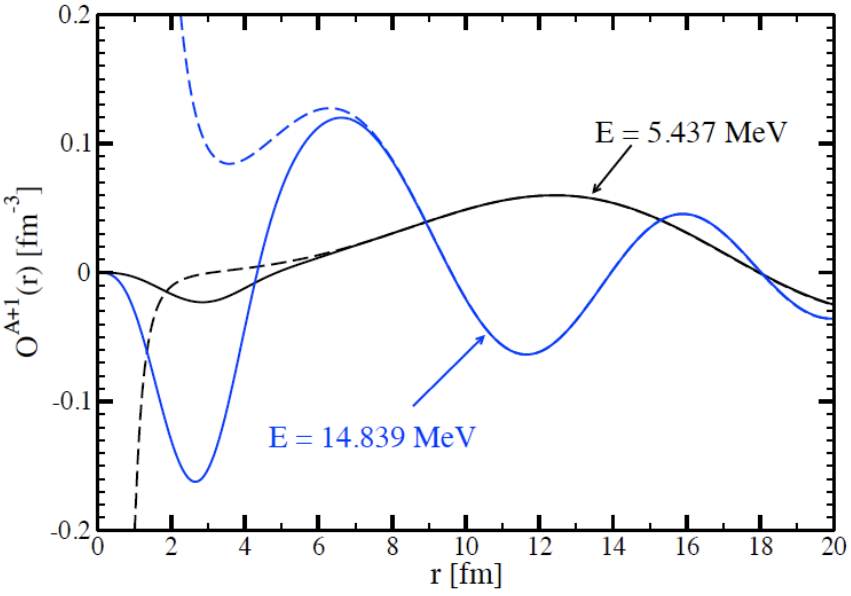
G. Hagen and N. Michel, Phys. Rev. C 86, 021602(R) (2012).

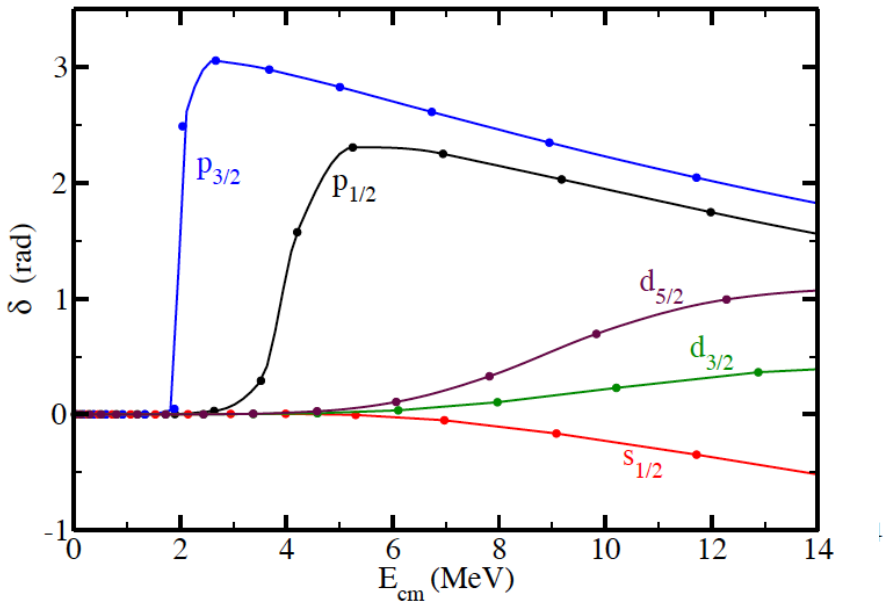
The one-nucleon overlap function: $O_A^{A+1}(lj;r) = \sum_n \langle A||a_{nlj}||A+1\rangle \phi_{nlj}(r)$

Beyond the range of the nuclear interaction the overlap functions take the form:

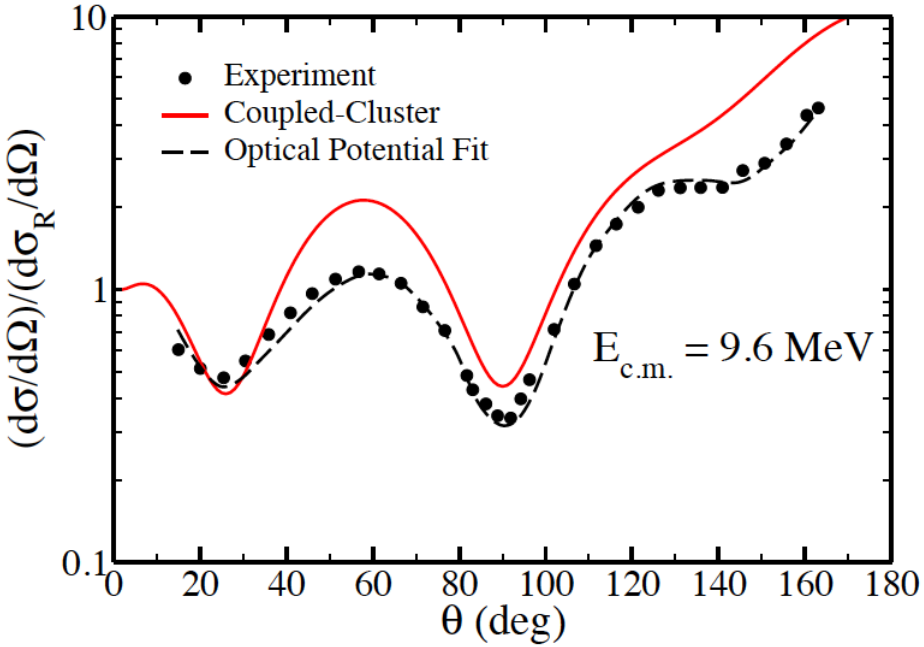
$$O_A^{A+1}(lj;kr) = C_{lj}\frac{W_{-\eta,l+1/2}(kr)}{r}, \quad k = i\kappa$$

$$O_A^{A+1}(lj;kr) = C_{lj}\left[F_{\ell,\eta}(kr) - \tan\delta_l(k) G_{\ell,\eta}(kr)\right]$$





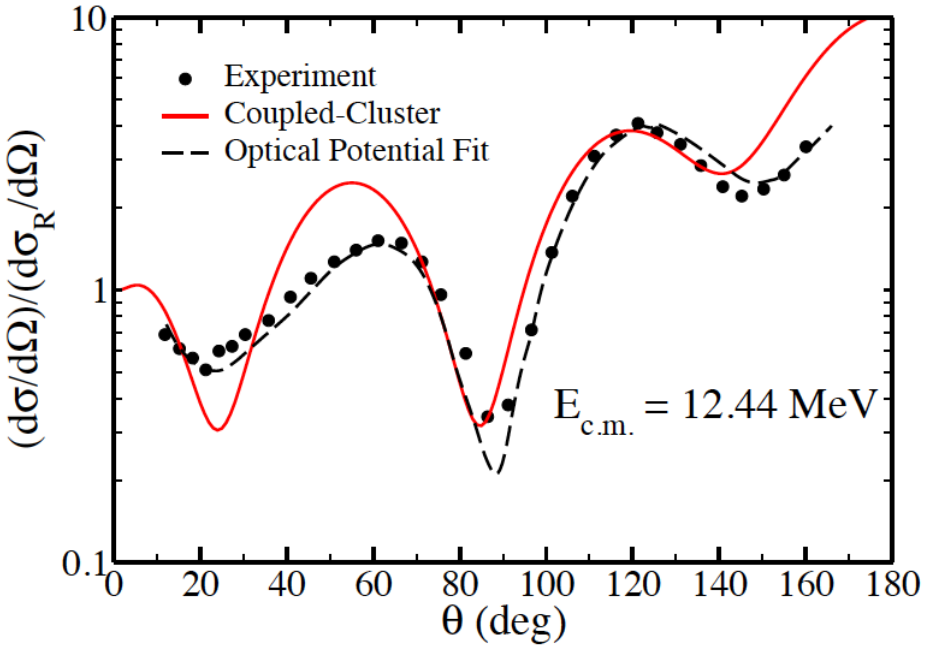
Elastic proton/neutron scattering on 40Ca



Differential cross section for elastic proton scattering on ^{40}Ca.

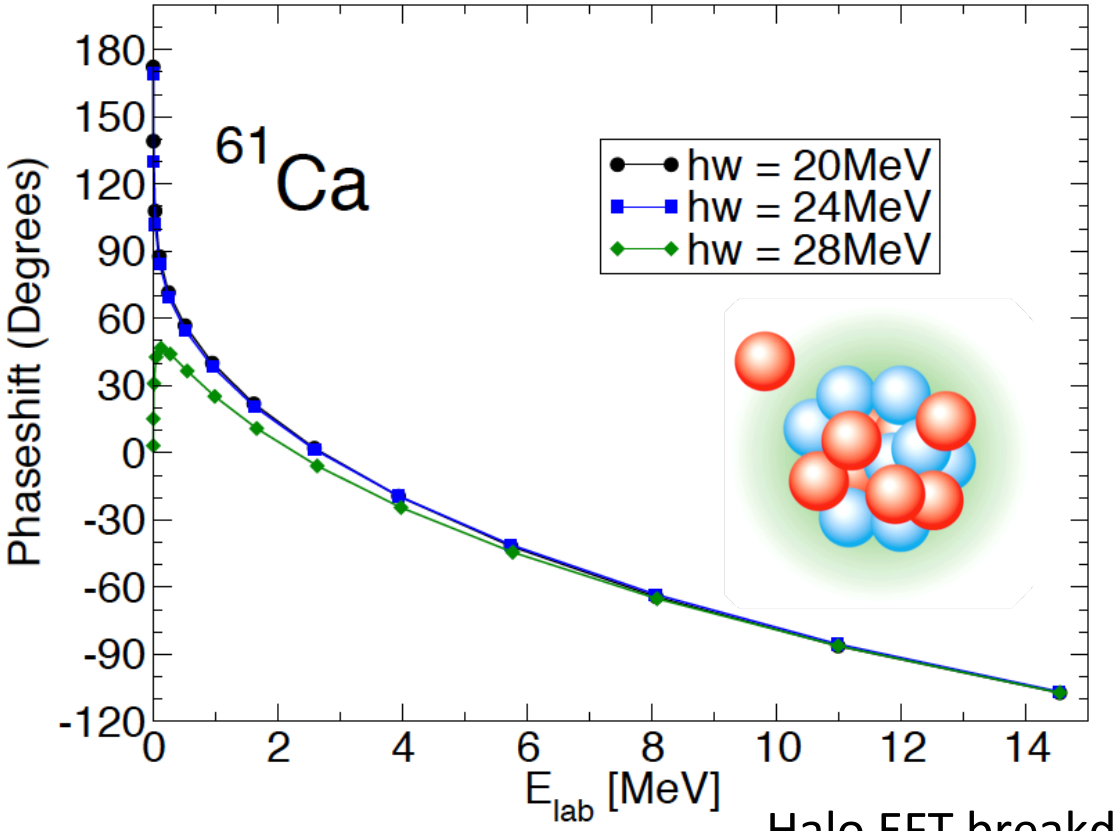
Fair agreement between theory and experiment for low-energy scattering.

G. Hagen and N. Michel
Phys. Rev. C **86**, 021602(R) (2012).



Efimov physics around neutron rich 60Ca

G. Hagen, P. Hagen, H.-W. Hammer, and L. Platter, PRL 111, 132501 (2013)



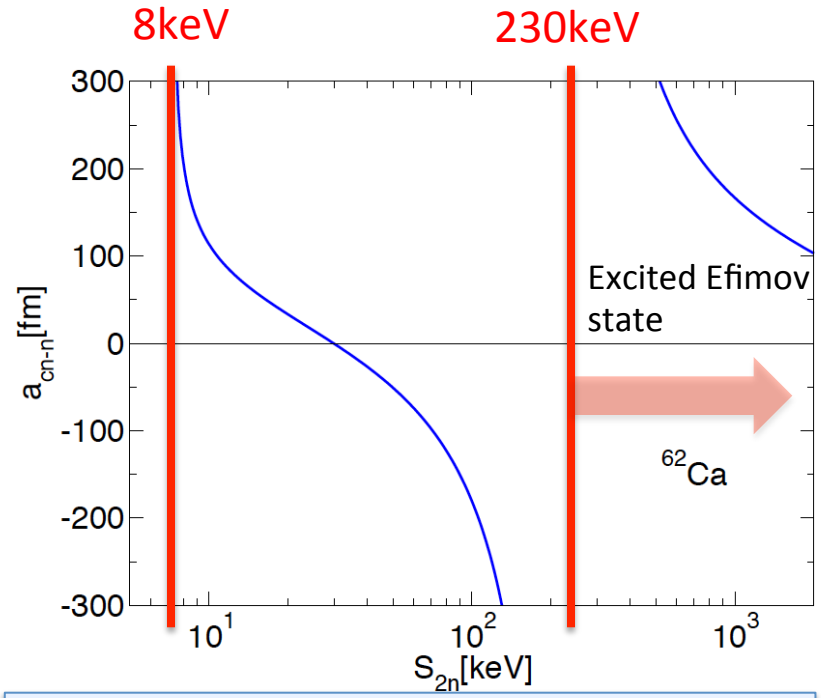
- Phase shifts from CC overlap functions
- Large S-wave scattering length in ^{61}Ca implies Halo phenomena
- Novel Approach: Merge halo-EFT and input from CC to study properties of ^{62}Ca

Halo EFT breakdown scale

$\hbar\omega$ [MeV]	a_{cn} [fm]	r_{cn} [fm]	S_n [keV]	S_{deep} [keV]
20	55.0	8.8	8.4	544
24	53.2	9.1	5.3	509
28	-26.1	10.8	-	361

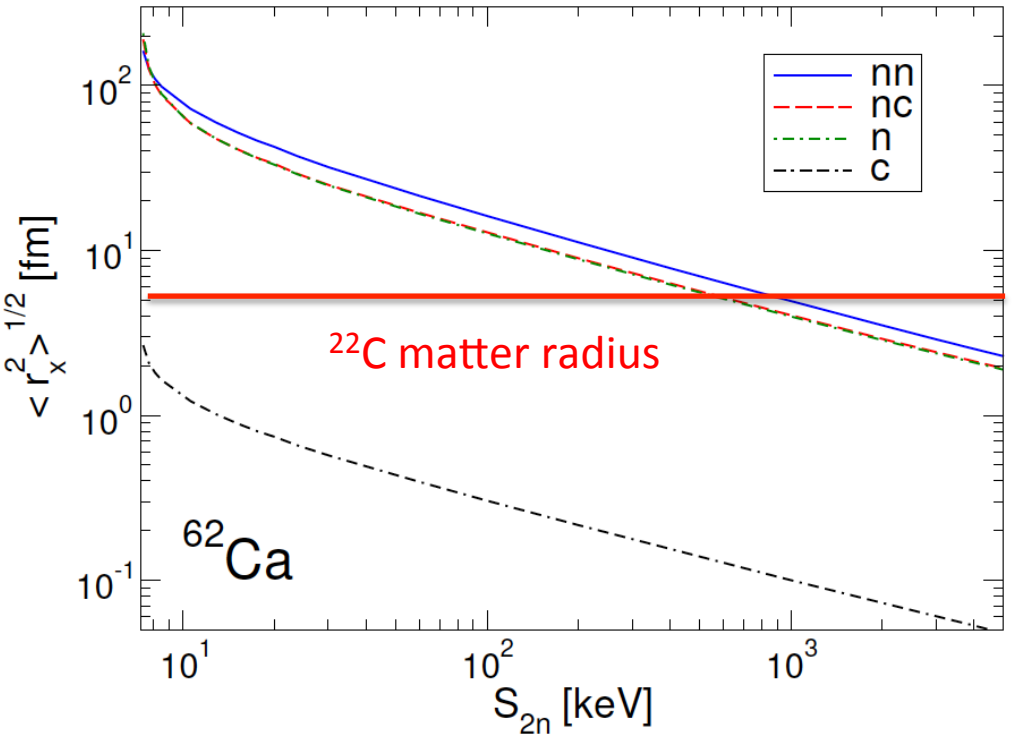
	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Efimov physics around neutron rich 60Ca



- For S_{2n} larger than ~ 230keV another state appears in the spectrum
- ^{62}Ca is likely to have an Efimov state (large halo)
- It is conceivable that ^{62}Ca displays an excited Efimov state

- ^{22}C is the largest known two-neutron halo R_{rms} ~5.4fm (Tanaka PRL 2010)
- Computed matter radii for ^{62}Ca indicates that it has the potential to be the largest and heaviest halo in the chart of nuclei



Nucleonic matter with forces from chiral EFT
[Hagen *et al.*, PRC 89 014319 (2013)]

- Use plane-wave basis with periodic boundary conditions

$$k_{n_i} = \frac{2\pi n_i}{L} \qquad n_i = 0, \pm 1, \pm 2, \ldots$$

- Yields closed shell "Fermi" spheres:

$$n = 1, 7, 19, 27, 33, 57, \ldots$$

- ☺ Basis respects momentum conservation
- ☺ Coupled clusters CCD (no singles) for closed-shell references
- ☺ Three-nucleon forces much simpler to implement than in shell-model basis

Related studies with chiral interactions: Soma & Bozek (2008); Epelbaum, Krebs, Lee, & Meissner (2009); Hebeler & Schwenk (2010); Hebeler, Bogner, Furnstahl, Nogga, & Schwenk (2011); Holt, Kaiser, & Weise (2012); Carbone, Polls, & Rios (2013); Gezerlis, Tews, Epelbaum, Gandolfi, Hebeler, Nogga, & Schwenk (2013); …

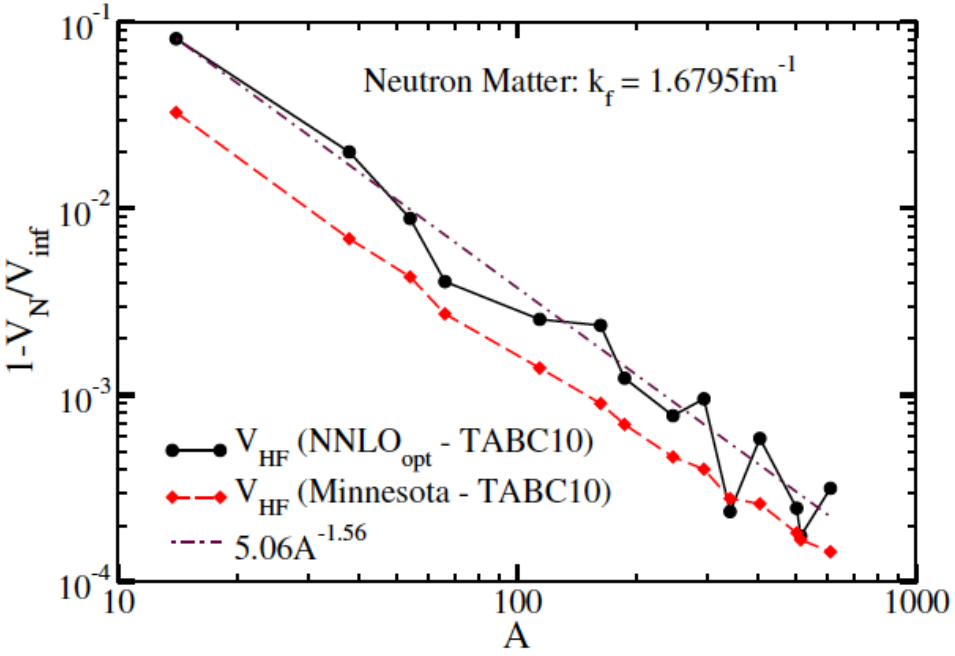
Mitigate shell oscillations

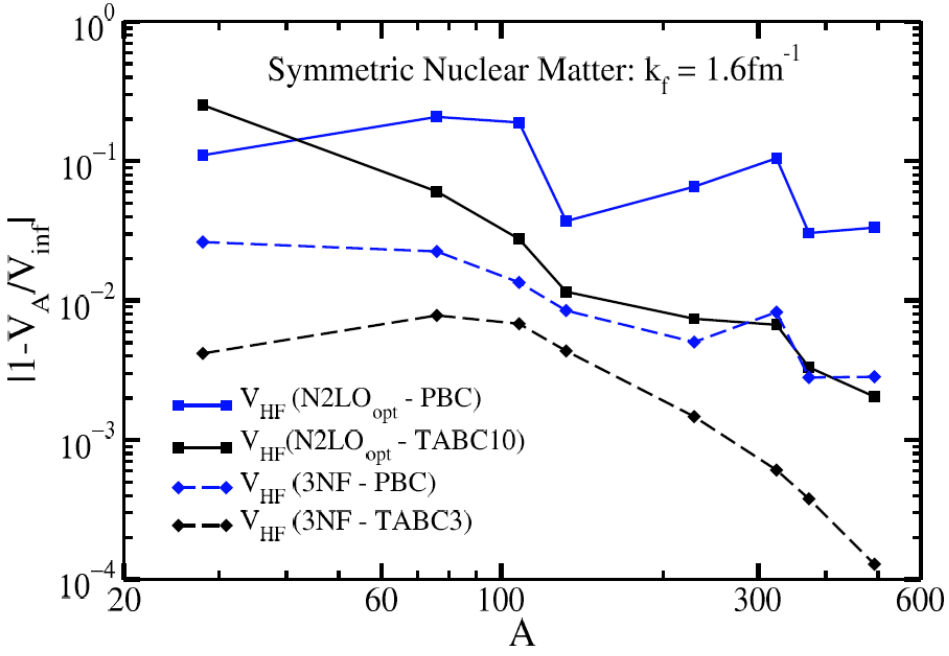
"Twist averaged" boundary conditions: average over all possible phases of Bloch waves. Exactly removes finite size effects for free Fermi gas:

$$\psi_k(x+L) = e^{i\theta}\psi_k(x) \qquad k_{n_i} = \frac{(2\pi n_i + \theta_i)}{L}$$

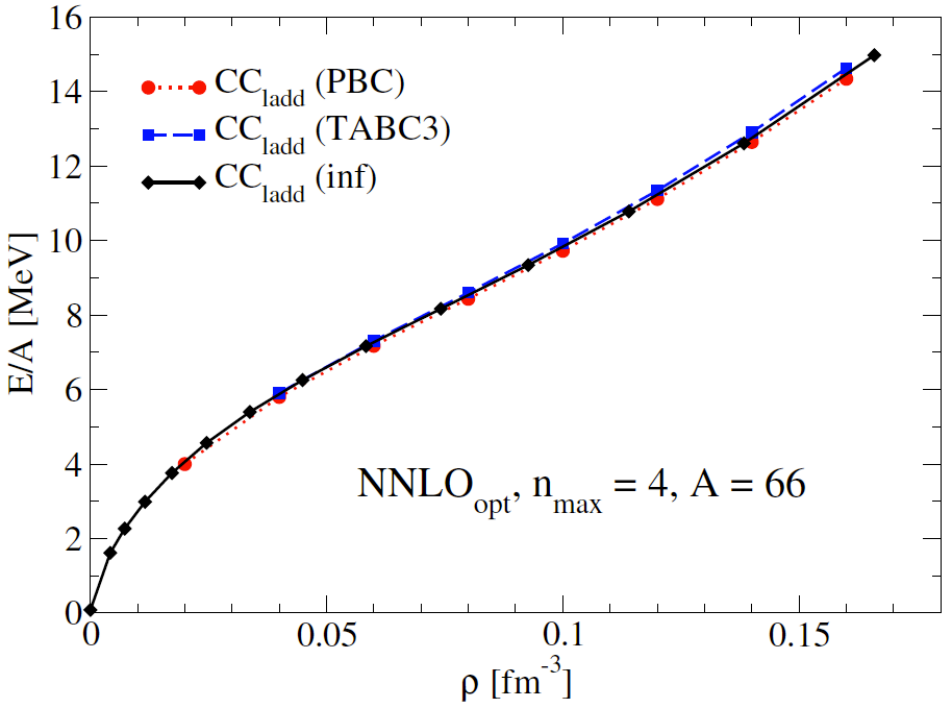
[Gros, Z. Phys. B 86, 359 (1992); Lin, Zong, and Ceperley, Phys. Rev. E 64, 016702 (2001)]
Discrete momenta are

Relative finite size corrections for the Hartree-Fock energy in nucleonic matter

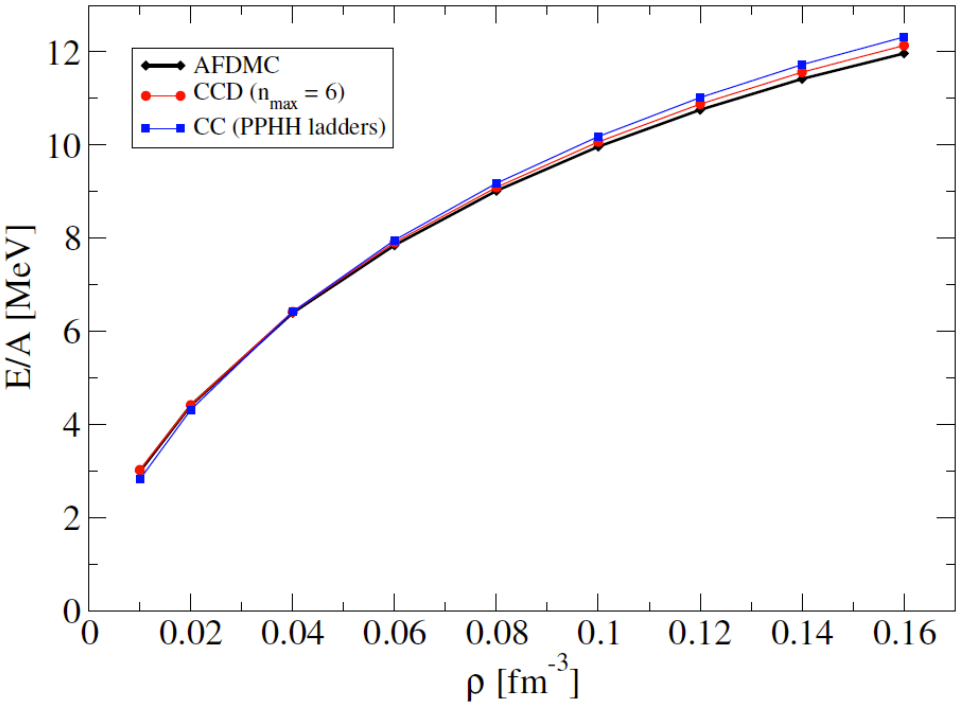




Benchmark calculations of neutron matter



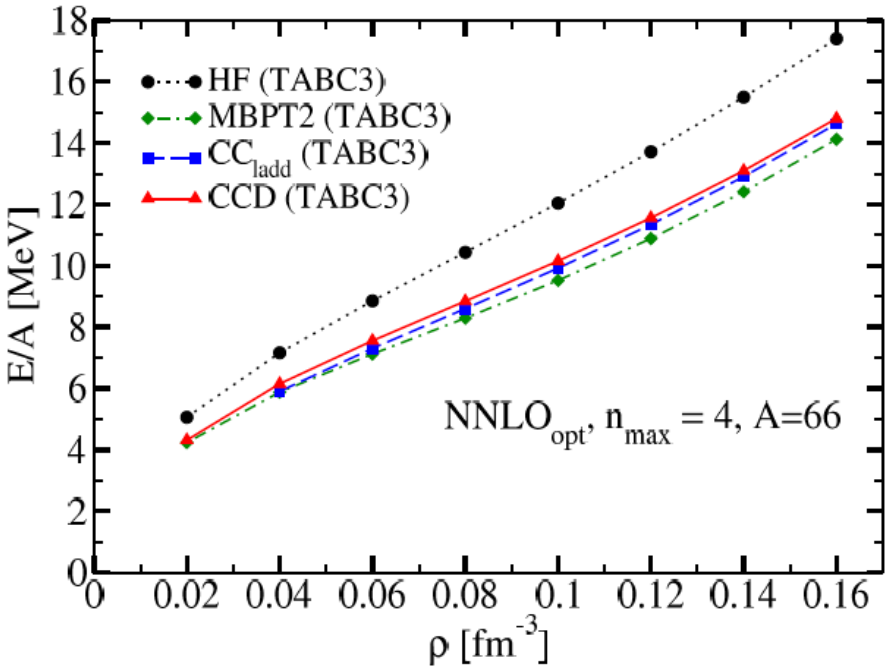
Comparison with continuum coupled-cluster method [Baardsen *et al.*, PRC (2013)]



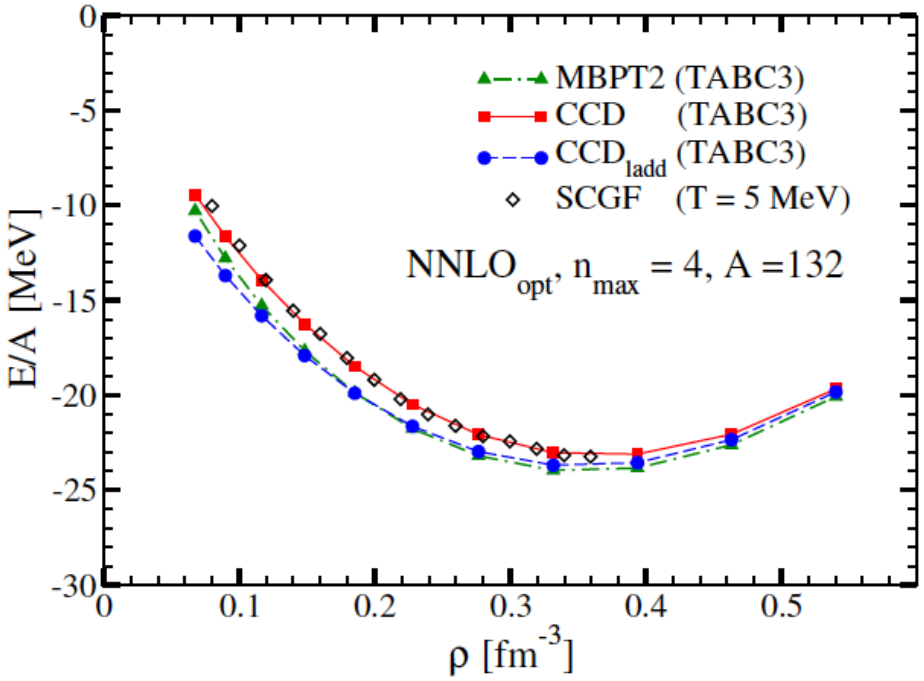
Comparison with auxiliary field diffusion Monte Carlo and Minnesota potential

Role of particle-hole excitations in nucleonic matter

Pure neutron matter (NN-only)



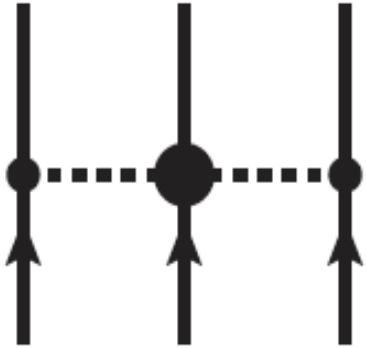
Symmetric nuclear matter (NN-only)



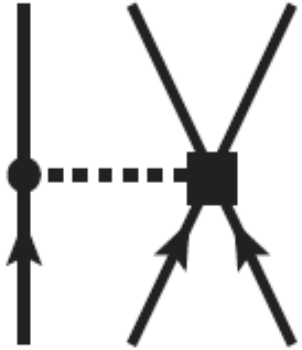
- Particle-hole and non-linear terms in CCD are small in pure neutron matter.
- MBPT2/CCD$_{ladd}$/CCD results agree within 500keV/A. Indicates that PNM is perturbative
- Particle-hole and non-linear terms play a larger role in symmetric nuclear matter.
- CCD$_{ladd}$ and CCD results differ by up to 1.5MeV/A around saturation density.

Three nucleon force (3NF) and regulator dependence

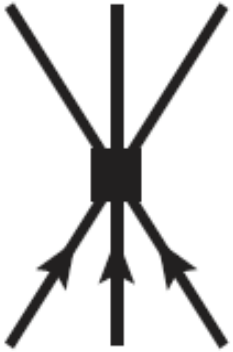
van Kolck, Phys. Rev. C 49, 2934 (1994); Epelbaum et al., Phys. Rev. C 66, 064001 (2002)



$c_{1,2,3}$



c_D



c_E

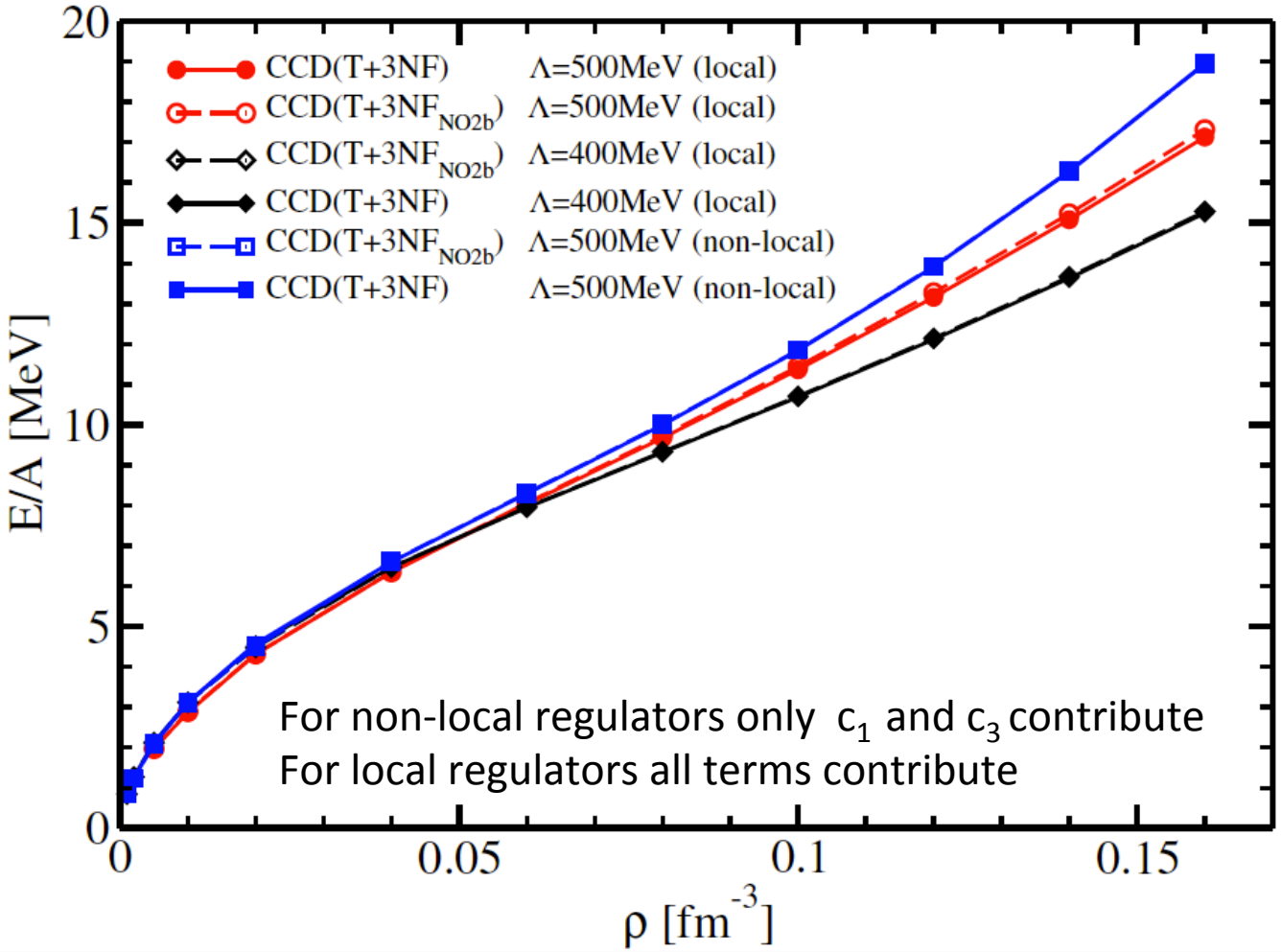
Nonlocal form of 3NF [Epelbaum et al. PRC (2002)]: Cutoff is in Jacobi momenta
Λ=500 MeV: c_D=-2, c_E=-0.791 (from A=3 binding energies)

Local form of 3NF [Navratil, Few Body Syst. (2007)]: Cutoff is in the momentum transfer

Λ=500 MeV: c_D=-0.39, c_E=-0.389 (from A=3,4 binding and ^{3}H $\tau_{1/2}$ (Gazit, Navratil, & Quaglioni)

Λ=400 MeV: c_D=-0.39, c_E=-0.27 (adjusted to ^{4}He)

Neutron matter

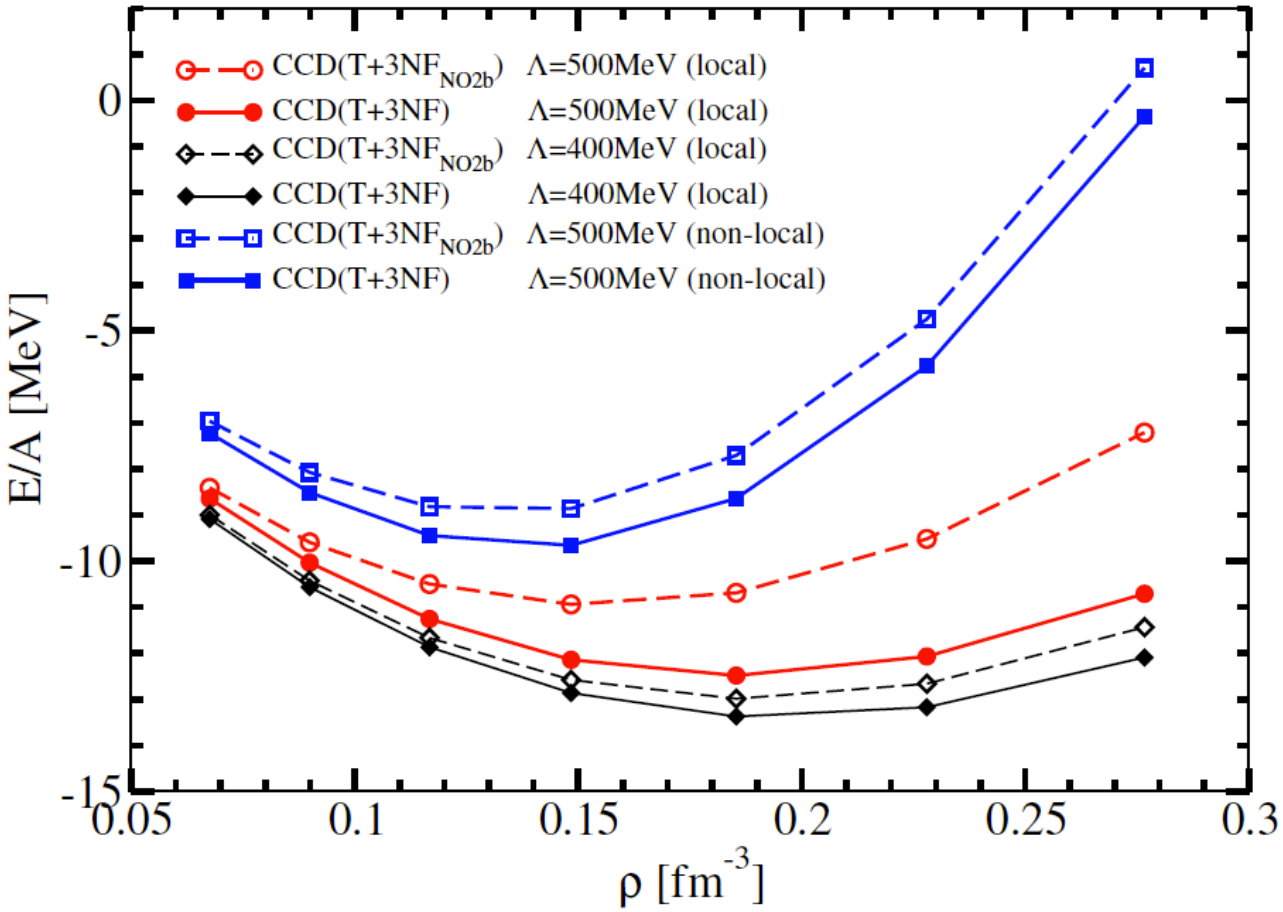


Neutron matter is perturbative (small differences between MBPT2 and coupled clusters

3NFs act repulsively in neutron matter and NNLO$_{opt}$

Error bands from variation of cutoffs and level of sophistication in treating 3NFs

Symmetric nuclear matter

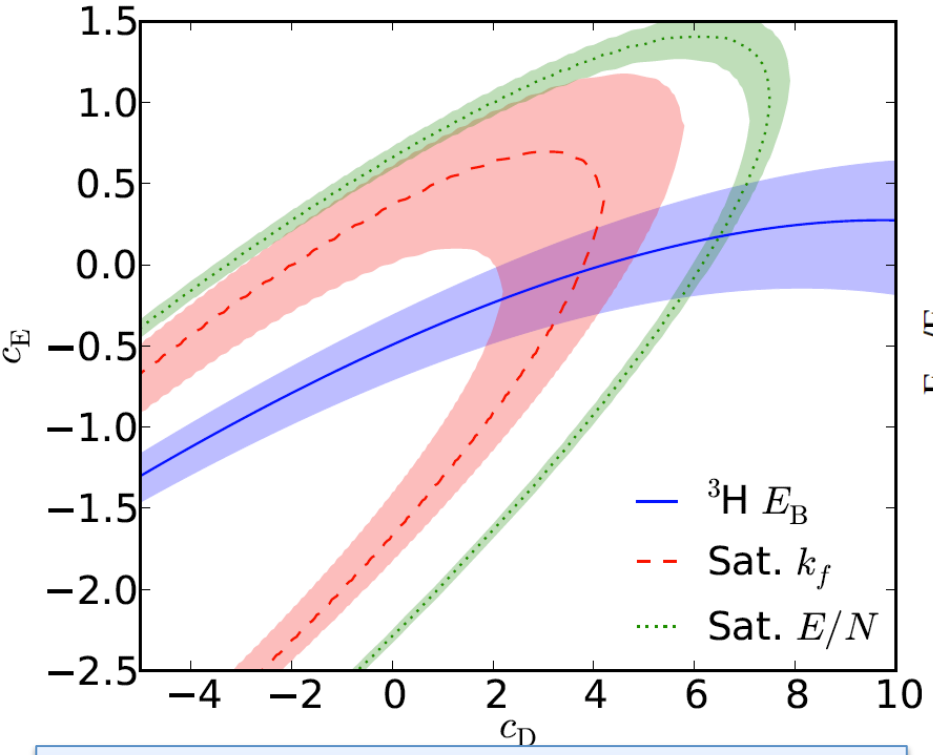


Nuclear matter is not perturbative (larger differences between MBPT2 and coupled clusters)

3NFs act repulsively in nuclear matter and NNLO$_{opt}$

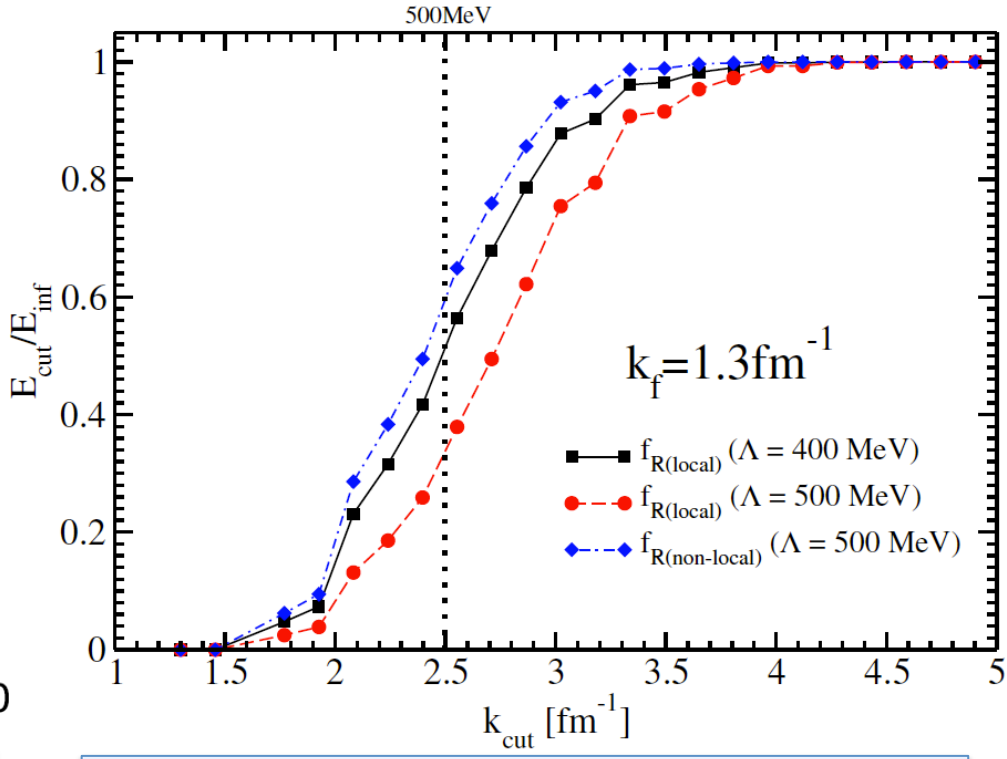
☹ Regularization scheme dependence of 3NF; sensitivity to sophistication in treatment of 3NFs

Understanding the 3NF at NNLO



5% error bands for saturation k_f, E/N and binding energy of ^{3}H

☹ Variation of c_D and c_E not sufficient to simultaneously bind light nuclei and nuclear matter



Cutoff dependent fraction of residual 3NF contribution to MBPT2 energy per particle in SNM around saturation density.

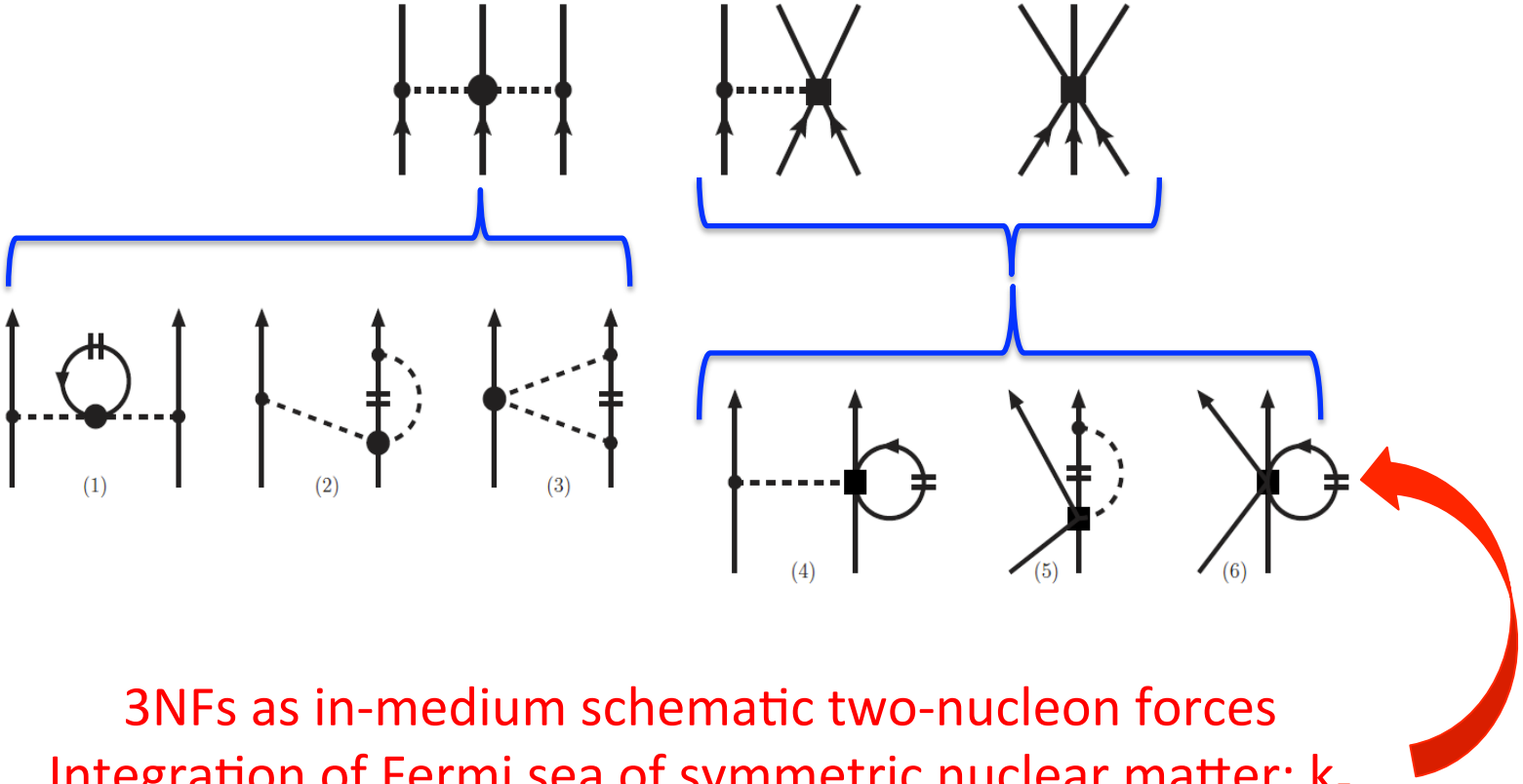
Local regulators converge slower than non-local regulators

Summary

1. Description of elastic scattering in medium mass nuclei from coupled-cluster theory.
2. Halo EFT with input from ab-initio coupled-cluster calculations. Description of universal properties in systems with large scattering length: Efimov physics in ^{62}Ca
3. Non-perturbative coupled-cluster computations of nucleonic matter with chiral NN and 3N interactions.
4. Not possible to obtain correct saturation properties of SNM and light nuclei simultaneously: include saturation point of SNM in optimization of chiral interactions.

Schematic Inclusion of 3NF effects

[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]



3NFs as in-medium schematic two-nucleon forces

Integration of Fermi sea of symmetric nuclear matter: k_F

Parameters: For Calcium we use $k_F = 0.95$ fm^{-1}, $c_E = 0.735$, $c_D = -0.2$ from binding energy of ^{40}Ca and ^{48}Ca (The contact parameter c_E differ from the value proposed for light nuclei)

Towards nuclear reactions with coupled-cluster theory

One-nucleon overlap functions

Elastic scattering, capture and transfer reactions of a nucleon on/to a target nucleus with mass A is determined by the one-nucleon overlap function

$$O_A^{A+1}(lj;r) = \sum_n \langle A||a_{nlj}||A+1\rangle \phi_{nlj}(r)$$

The left ground-state for target nucleus A is given by: $\langle A| = \langle \Phi_0|L_0 e^{-T}$

$$\langle \Phi_0|L_0 e^{-T} H e^{T} = \langle \Phi_0|L_0 \bar{H} = E_0 \langle \Phi_0|$$

The A+1 final states are computed via particle-attached coupled-cluster method:

$$|A+1\rangle = R^{A+1} e^{T} |\Phi_0\rangle = e^{T} \left(\sum_a r^a a_a^\dagger + \frac{1}{2} \sum_{abi} r_i^{ab} a_a^\dagger a_b^\dagger a_i \right) |\Phi_0\rangle$$

$$\bar{H} R^{A+1} |\Phi_0\rangle = E^{A+1} R^{A+1} |\Phi_0\rangle$$

Towards nuclear reactions with coupled-cluster theory

One-nucleon overlap function from coupled cluster theory:
Ø. Jensen et al PRC 82, 014310 (2010).

$$O_A^{A+1}(lj;r) = \sum_n \langle \Phi_0 | L_0 \overline{a_{nlj}} R^{A+1} | \Phi_0 \rangle \phi_{nlj}(r)$$

Bergren basis
ensures correct asymptotic behavior

The similarity transformed annihilation/creation operator calculated via the Baker-Campbell-Hausdorff commutator expansion:

$$\overline{a_p} = e^{-T} a_p e^T = [a_p, T]$$

$$\overline{a_p} = a_p + \sum_i t_i^p a_i + \frac{1}{2} \sum_{ijc} t_{ij}^{pc} a_c^\dagger a_j a_i$$

Treatment of long-range Coulomb effects

The A-nucleon Hamiltonian is:

$$\hat{H} = \sum_{1 \le i < j \le A} \left(\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \hat{V}_{NN}^{(i,j)} + \hat{V}_{\text{Coul}}^{(i,j)} + \hat{V}_{\text{3Neff}}^{(i,j)} \right)$$

We add and subtract a one-body Coulomb term:

$$V_{\text{Coul}} = U_{\text{Coul}}(r) + [V_{\text{Coul}} - U_{\text{Coul}}(r)]$$

$$U_{\text{Coul}}(r) \longrightarrow (Z-1)e^2/r \text{ for } r \to +\infty$$

We construct the Coulomb Berggren basis by diagonalizing the 1-body Schrodinger equation In a basis of spherical Bessel functions:

$$h = \frac{\hat{p}^2}{2m} - V_o \left[1 + \exp\left(\frac{r - R_0}{d} \right) \right]^{-1} + U_{\text{Coul}}(r)$$

Numerical example: proton resonances in ^{17}F In a Woods-Saxon potential

		$s_{1/2}$		$d_{3/2}$		$d_{5/2}$	
N_R	N_T	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
5	15	1.1054	0.1446	5.0832	1.3519	1.4923	0.0038
5	20	1.1033	0.1483	5.0785	1.3525	1.4873	0.0079
10	25	1.0989	0.1360	5.0765	1.3525	1.4858	0.0093
10	30	1.0986	0.1366	5.0757	1.3529	1.4849	0.0103
15	40	1.0978	0.1351	5.0749	1.3531	1.4842	0.0111
15	50	1.0978	0.1353	5.0746	1.3533	1.4838	0.0114
20	60	1.0976	0.1349	5.0745	1.3533	1.4837	0.0116
30	70	1.0975	0.1346	5.0744	1.3534	1.4837	0.0117
(Michel 2011)		1.0975	0.1346	5.0744	1.3535	1.4836	0.0119

The one-body coulomb potential has a Logarithmic singularity at $Q_l(1)$:

$$U_{\text{Coul}}(k,k') = \langle k | U_{\text{Coul}}(r) - \frac{(Z-1)e^2}{r} | k' \rangle + \frac{(Z-1)e^2}{\pi} Q_\ell \left(\frac{k^2 + k'^2}{2kk'} \right)$$

The singularity is removed by **the off-diagonal method**: replace the singularity by a finite value depending on the quadrature

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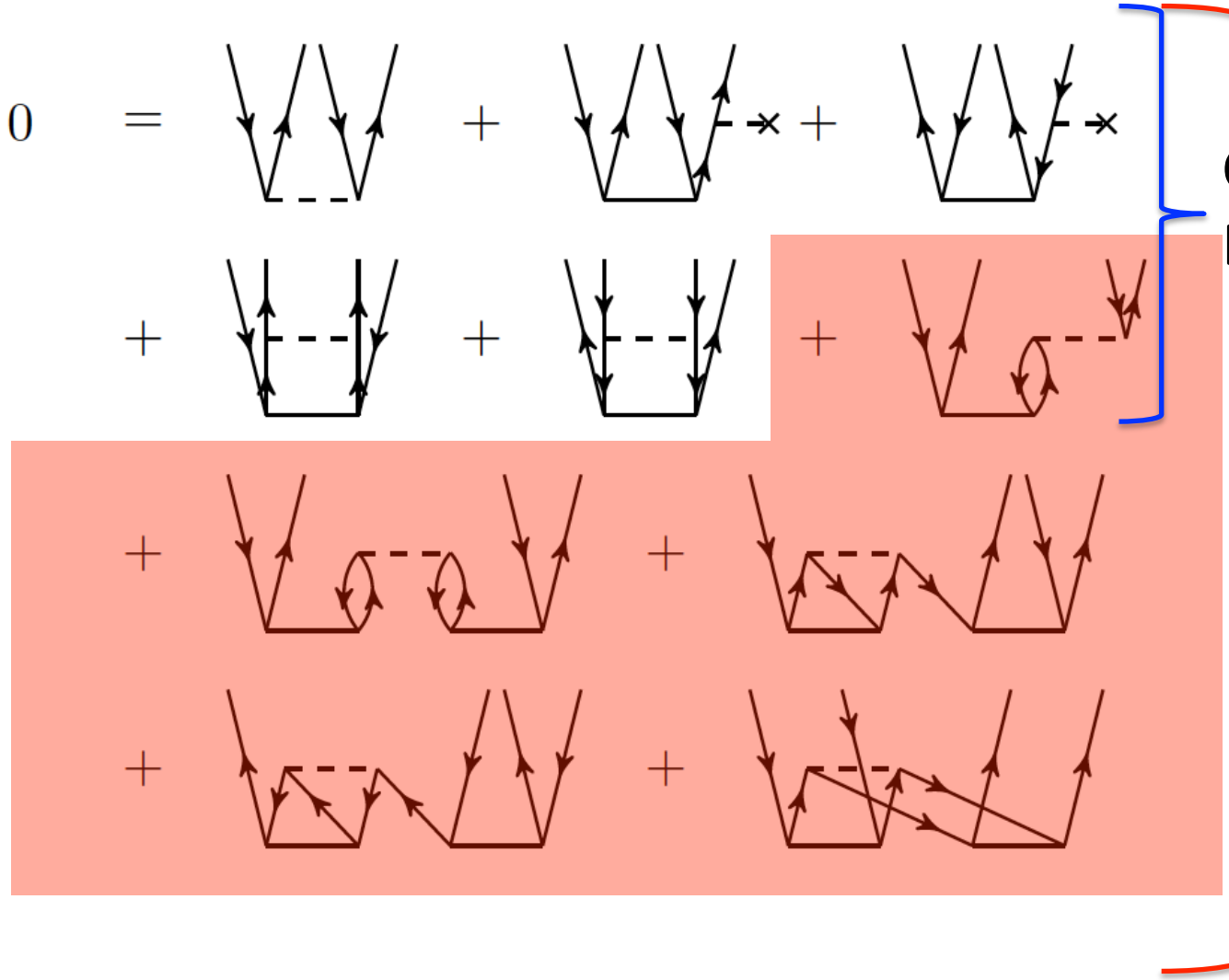
Efimov physics around neutron rich 60Ca

- Halo EFT provides a model-independent description of halo nuclei
- Core + valence nucleons are effective degrees of freedom
- The coupling constants from the *n-n* and core-*n* effective range
- The expansion is given in powers of R/a with R ~ effective range
- Use coupled-cluster results for ^{61}Ca to study signals of Efimov physics

The Halo EFT core *n-n* Lagrangian to leading order:

$$\begin{aligned}\mathcal{L} &= \psi_c^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{2M} \right) \psi_c + \vec{\psi}_n^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{2m} \right) \vec{\psi}_n \\ &+ \Delta_{nn}\, d_{nn}^\dagger d_{nn} + \Delta_{cn}\, \vec{d}_{cn}^\dagger \vec{d}_{cn} + h\, d_{nn}^\dagger \psi_c^\dagger \psi_c\, d_{nn} \\ &- \left[g_{cn}\, \vec{d}_{cn}^\dagger \vec{\psi}_n\, \psi_c + \frac{g_{nn}}{2} d_{nn}^\dagger \left(\vec{\psi}_n^{\,\mathrm{T}} P\, \vec{\psi}_n \right) + \mathrm{h.c} \right] + \dots \ .\end{aligned}$$

Coupling constants given by *n-n* and core-*n* effective ranges

Three-body coupling

Infinite matter from Coupled-Cluster Theory