Lawrence Livermore National Laboratory

Towards a fundamental understanding of light nuclei and their low-energy reactions

Sofia Quaglioni (LLNL), Petr Navratil (LLNL), and Doron Gazit (INT)

Effective Field Theories and the Many-Body Problem

INT 09-1, Seattle, March 24, 2009

Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, CA 94551

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

LLNL-PRES-411494

Outline

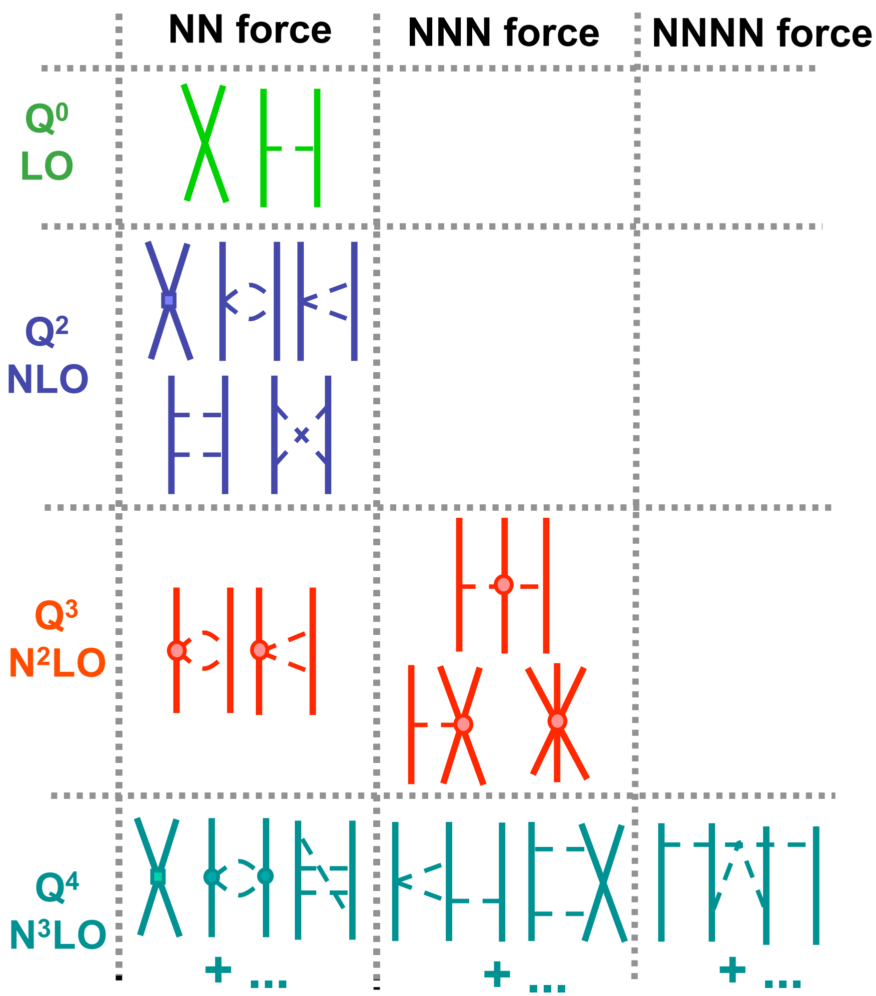
The advancement in the determination of the inter-nucleon interactions strives on the progress of the ab initio description of nuclei and vice versa

- Part I
  - Three-nucleon low-energy constants from the consistency of interactions and currents in chiral effective field theory
    - in collaboration with Doron Gazit and Petr Navratil

- Part II
  - *Ab initio* many-body calculations of nucleon-nucleus scattering
    - in collaboration with Petr Navratil

A new generation of nuclear interactions (and currents)

- Nuclear forces are governed by quantum chromodynamics (QCD)
  - QCD non perturbative at low energies
- Chiral effective filed theory (χEFT)
  - retains all symmetries of QCD
  - explicit degrees of freedom: π, N
- Perturbative expansion in positive powers of $(Q/\Lambda_\chi)\ll 1$ ($\Lambda_\chi \sim$ 1 Gev)
  - nuclear interactions
  - nuclear currents
- Chiral symmetry dictates operator structure
- Low-energy constants (LECs) absorb short-range physics
  - some day all from lattice QCD
  - now constrained by experiment

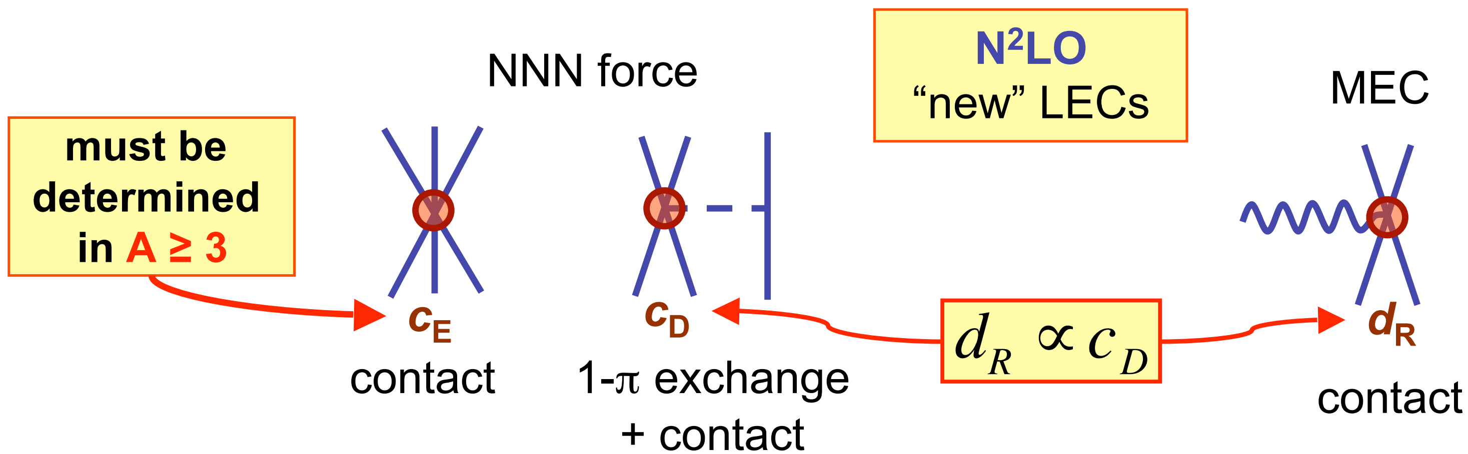


Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

Challenge and necessity: apply χEFT forces to nuclei

χEFT NN + NNN interactions and currents

- A high precision fit to NN data is reached at order N^{3}LO in the chiral expansion
  - N^{3}LO NN [Entem&Machleidt, PRC **68**, 041001 (2003); Epelbaum *et al.*, NPA **747**, 362 (2005)]
- Nuclear current [Park *et al.*, PRC **67**, 055206 (2003); Gazit, PLB **666**, 472 (2008)]
  - LO: standard single-nucleon terms
  - N^{2}LO: first appearance of meson-exchange current (MEC)
- Up to N^{3}LO both potential and current are fully constrained by the parameters defining the NN interaction, with the exception of two "new" LECs, c_E and c_D



Link between medium-range NNN force (c_D term) and MEC in nuclear β-decay

Triton half life

- The ^3H is an unstable nucleus, which undergoes β-decay
  - Simpson, PRC **35**, 752 (1987); Schiavilla *et al.*, PRC 58, 1263 (1998)

kinematical factor over vector coupling constant

Small difference in statistical rate functions

$$(fT_{1/2})_t = \frac{K/G_V^2}{(1-\delta_c) + 3\pi \frac{f_A}{f_V} \langle E_1^A \rangle^2}$$

"comparative" half life
$(fT_{1/2})_t = 1129.6 \pm 3\ s$
PLB **610**, 45 (2005)

$\left| \langle {}^3He \| F \| {}^3H \rangle \right|^2$

$\delta_c = 0.13\%$ effect of isospin-breaking

$\left| \langle {}^3He \| E_1^A \| {}^3H \rangle \right|^2$

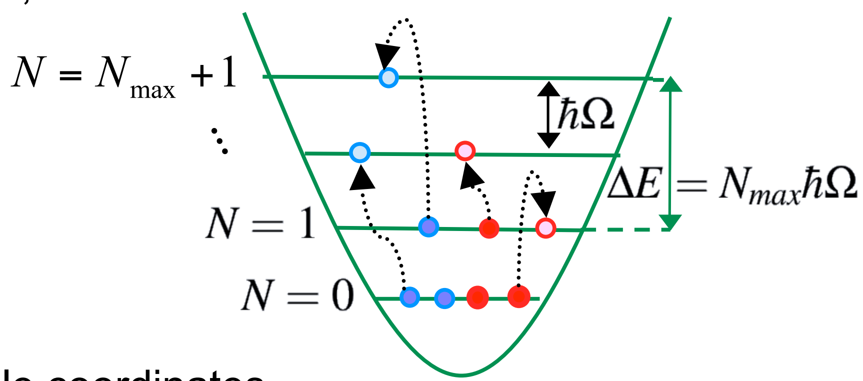
N.B.: $E_1^A \big|_{LO} \propto GT$

- Extract the phenomenological value of $\langle E_1^A \rangle \big|_{\exp t} = 0.6848 \pm 0.0011$

The *ab initio* no-core shell model (NCSM) in brief

The NCSM is a technique for the solution of the *A*-nucleon bound-state problem

- Hamiltonian
  - "realistic" (= reproduce NN data with high precision) NN potentials:
    - coordinate space: Argonne …
    - momentum space: CD-Bonn, χEFT N^{3}LO, …
  - NNN interactions:
    - Tucson-Melbourne TM', χEFT N^{2}LO



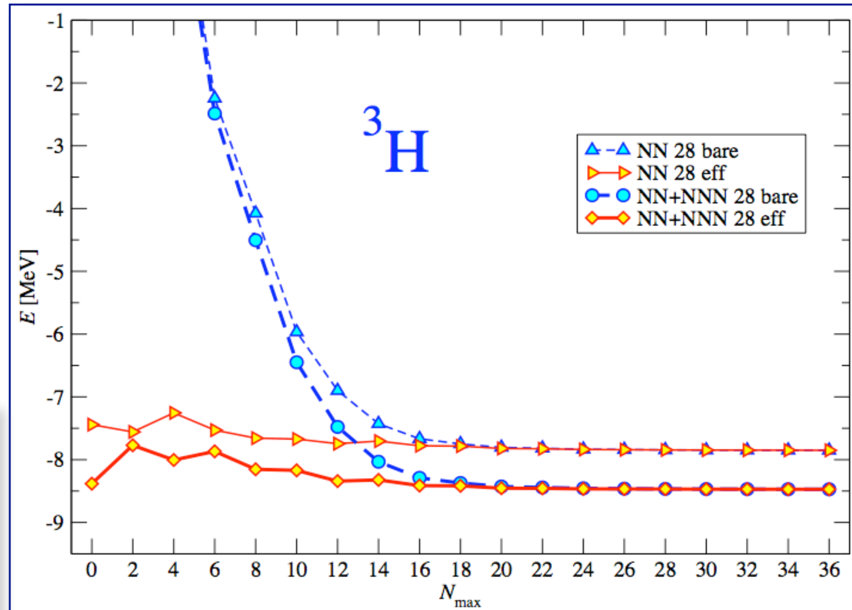
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
    - Jacobi relative **or** Cartesian single-particle coordinates
  - complete $N_{max}\hbar\Omega$ model space
    - translational invariance preserved even with Slater-determinant (SD) basis

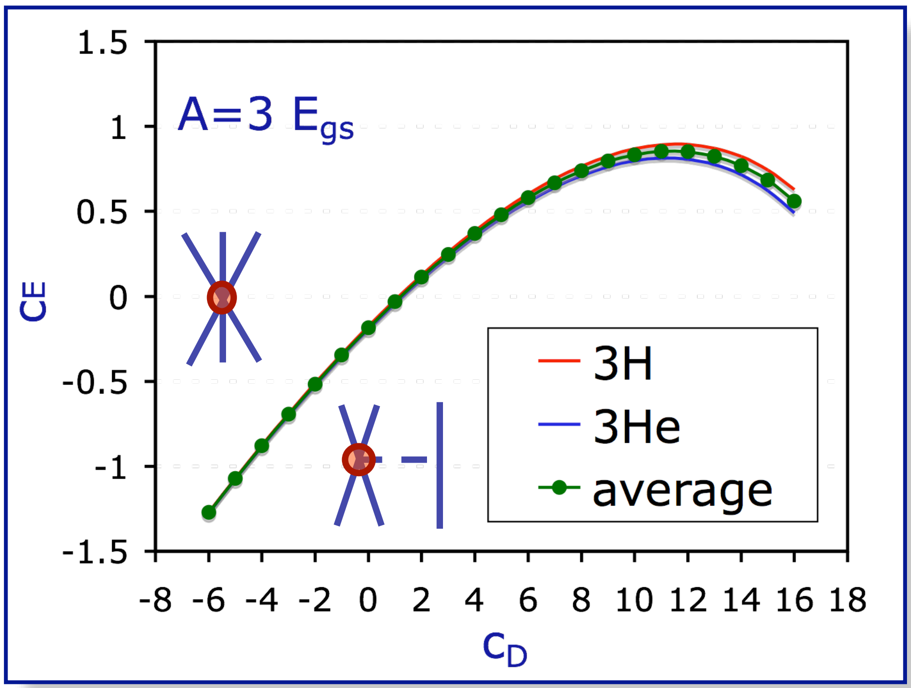
- Constructs effective interaction tailored to model-space truncation
  - unitary transformation in a *n*-body cluster approximation (*n*=2,3)

Convergence to exact solution with increasing N_{max}

Fit $c_{D,}c_E$ to experimental binding energy of ^{3}H (^{3}He)

- NCSM calculations in Jacobi coordinates
  - N^3LO NN (Entem & Machleidt), (two-body effective interaction)
  - N^2LO NNN (bare)

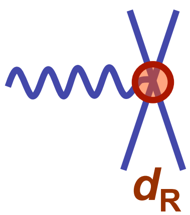




- There is an infinite number of c_D-c_E combinations that fit the A=3 b.e.
- Next: determine for wich c_D along the trajectory the calculated $\langle E_1^A \rangle$ reproduces $\langle E_1^A \rangle_{expt}$

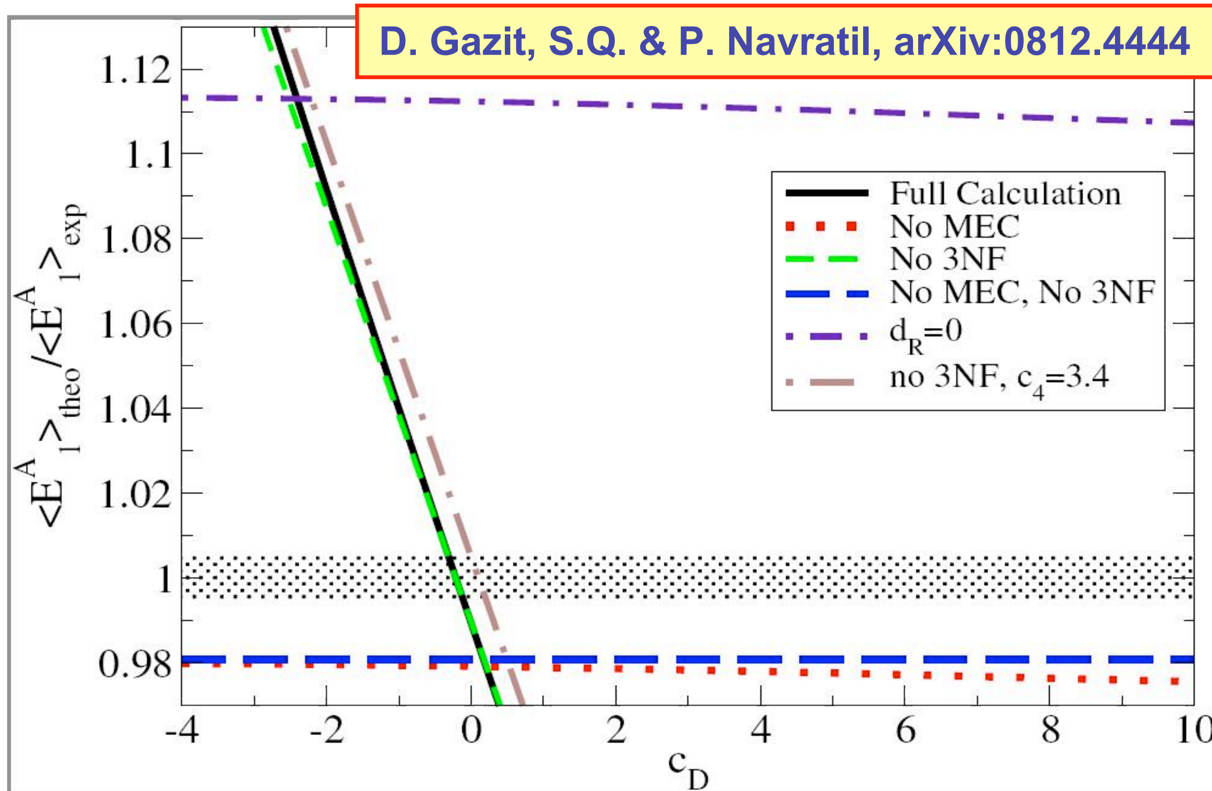
E_1^A reduced matrix element from χEFT

- LO: $\left. E_1^A \right|_{LO} \propto GT$
- N^2LO: MEC
  - One (charged) pion exchange term
  - contact term



$$d_R = \frac{M_N}{\Lambda_\chi g_A} c_D + \frac{M_N}{3}\left(c_3 + 2c_4\right) + \frac{1}{3}$$

D. Gazit, S.Q. & P. Navratil, arXiv:0812.4444



- NCSM calculation in Jacobi coordinates: N^3LO NN (Entem&Machleidt) + N^2LO NNN
  - MEC essential (especially contact term!)
  - weak sensitivity to NNN force
  - somewhat sensitive to c_3 and c_4

The half-life of Triton is a robust 2nd constraint!

Conclusions

- Chiral symmetry of QCD: link between electroweak processes and NNN-force
  - χEFT: c_D both in NN-π-N part of NNN force and contact term of MEC (Hanhart *et al*., Gårdestig & Phillips)
- Triton β-decay could be used to fix the NNN force (Gårdestig & Phillips)
- *Ab initio* NCSM calculations with N^3LO NN (Entem & Machleidt) + N^2LO NNN
  - we have shown that the Triton half-life is a robust second constraint
- Point of view of many-body theory:
  - Treat N^3LO NN (Entem & Machleidt) as phenomenological model
  - ➔ we have constrained the "corresponding" N^2LO NNN force
- Point of view of chiral effective filed theory:
  - To do: study cutoff dependence, clarify role of c_3 and c_4
  - ➔ more work ahead: determination of c_D, c_E not yet conclusive
- Work underway: *ab initio* NCSM calculations with N^3LO NN (Epelbaum *et al*.)
  - study cutoff dependence; clarify role of c_3 and c_4

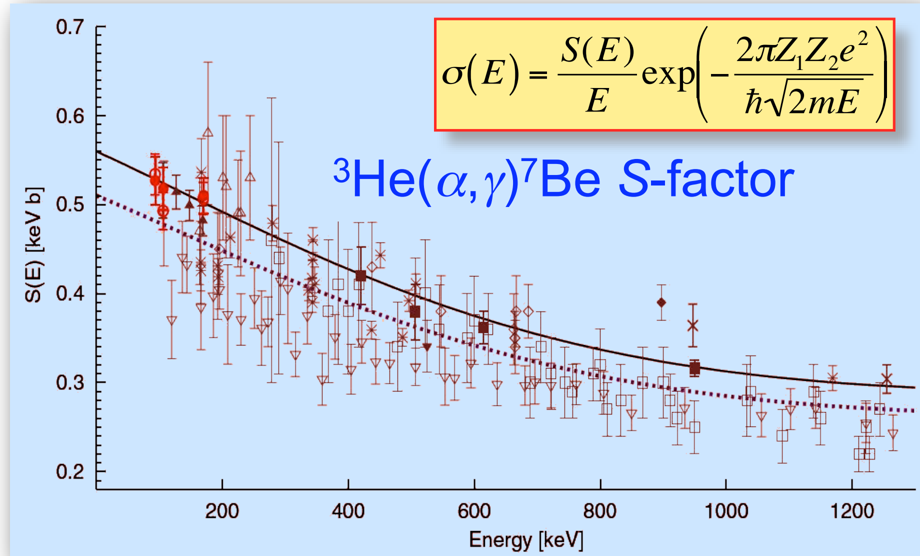
Outline

The advancement in the determination of the inter-nucleon interactions strives on the progress of the ab initio description of nuclei and vice versa

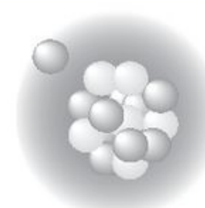
- Part I
  - Three-nucleon low-energy constants from the consistency of interactions and currents in chiral effective field theory
    - in collaboration with Doron Gazit and Petr Navratil
- Part II
  - *Ab initio* many-body calculations of nucleon-nucleus scattering
    - in collaboration with Petr Navratil

Nuclear foundations of astrophysics, experimental research on exotic nuclei, … formidable challenges to nuclear theory

- Astrophysics needs detailed and accurate nuclear physics inputs
  - low-energy reactions very difficult or impossible to measure
    - low rates due to Coulomb repulsion
    - energies relevant to astrophysics hard to reach in laboratory
    - electron screening can be large
  - extrapolations into regions in which experimental data are absent have uncertainties that are not quantifiable



- Exotic nuclei bring new phenomena to the forefront
  - weak binding, coupling to the continuum, extreme isospin
  - nucleon halos and skins, clustering
  - vanishing of magic numbers, abnormal spin-parity of ground states



"Nuclear theory has to go beyond its empirical roots , and arrive at a fundamental understanding of nuclear properties from a unified theoretical standpoint rooted in the fundamental forces among nucleons" RIA Theory Bluebook, 2005

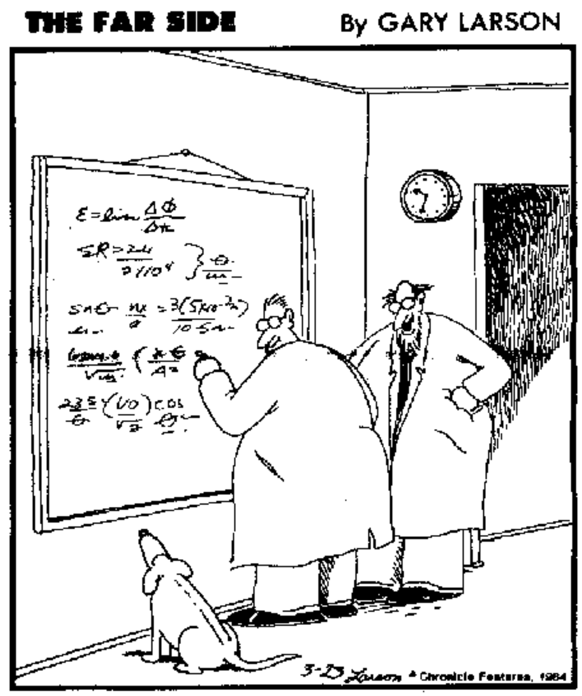
Our goal is to develop an *ab initio* approach to light nuclei and their low-energy reactions

- *Ab initio*, literally “from the beginning”, meaning:
  - non-relativistic quantum mechanics
  - *A* (active) point-like nucleons
  - realistic two- and three-nucleon forces (NN+NNN)

- A great deal of progress in *ab initio* nuclear structure
  - nuclei up to ***A*=16** and beyond (mostly well-bound)
  - provide insight on the role of the NNN force

- Now we need to extend the *ab initio* effort to describe
  - Nuclear reactions

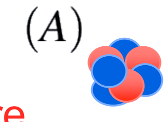
  ➔ many-body quantum-mechanical problem in the continuum. Even more challenging!
    - accurate nuclear reaction calculations for ***A*=3,4**
    - many-body scattering calculations for **A>4** only now under development
  - weakly-bound systems
    - need coupling of structure and reaction mechanisms

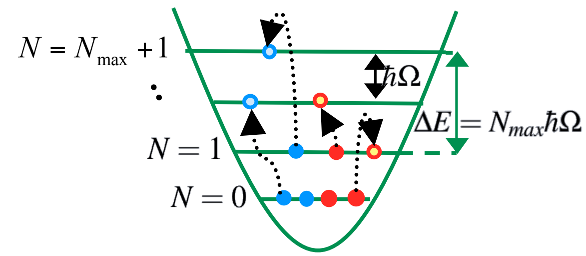


“Ohhhhhhh . . . Look at that, Schuster . . . Dogs are so cute when they try to comprehend quantum mechanics.”

Combining the *ab initio* no-core shell model (NCSM) and the resonating-group method (RGM) - *ab initio* NCSM/RGM

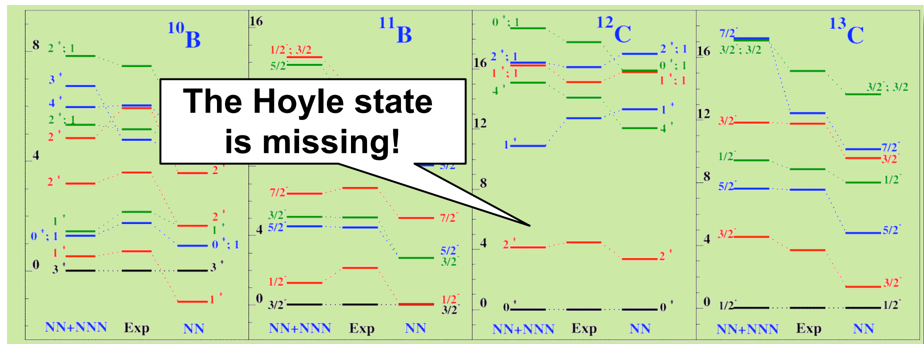
- NCSM - single-particle degrees of freedom





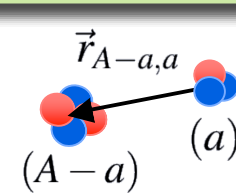
  - a successful *ab initio* approach to nuclear structure
  - for *A*>4, the only capable of employing QCD-based NN and NNN interactions derived within effective-field theory

  - incorrect description of wave function asymptotic ($r > 5$ fm)
  - lack of coupling to the continuum

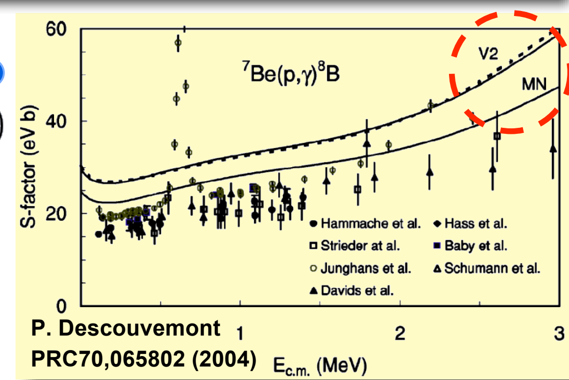


- RGM - clusters and their relative motion

  - a successful microscopic-cluster technique
  - preserves Pauli principle



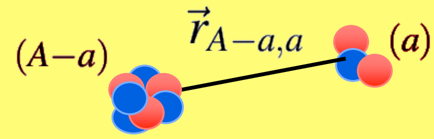
  - describes reactions and clustering in light nuclei
  - simplified NN interactions and internal description of clusters
  - no link to fundamental interactions among nucleons



- NCSM/RGM - RGM + realistic interactions + consistent description of clusters
  - *ab initio* description of both bound and scattering states in light nuclei

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$



$\psi^{(A-a)}_{1\nu}\, \psi^{(a)}_{2\nu}\, \delta(\vec{r} - \vec{r}_{A-a,a})$

eigenstates of $H_{(A-a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

$$H\Psi^{(A)} = E\Psi^{(A)}$$

$T_{\mathrm{rel}}(r) + \mathcal{V}_{\mathrm{rel}} + \bar{V}_{\mathrm{Coul}}(r) + H_{(A-a)} + H_{(a)}$

either bare interaction or NCSM effective interaction

$$\sum_{\nu} \int d\vec{r} \left[\mathcal{H}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) - E\,\mathcal{N}^{(A-a,a)}_{\mu\nu}(\vec{r}\,', \vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$

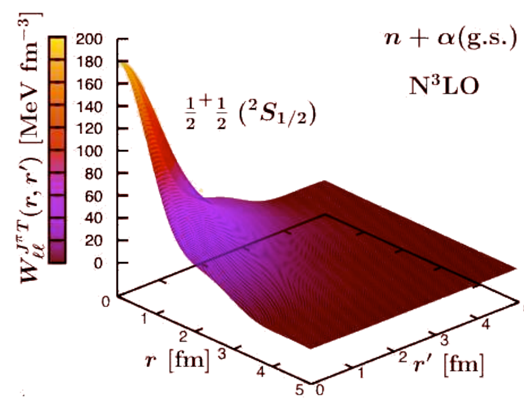
Hamiltonian kernel

$\langle \Phi^{(A-a,a)}_{\mu\vec{r}\,'} | \hat{\mathcal{A}}^2 | \Phi^{(A-a,a)}_{\nu\vec{r}} \rangle$

Norm kernel

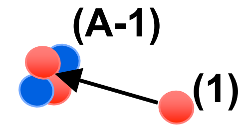
- Non-local integro-differential coupled-channel equations:

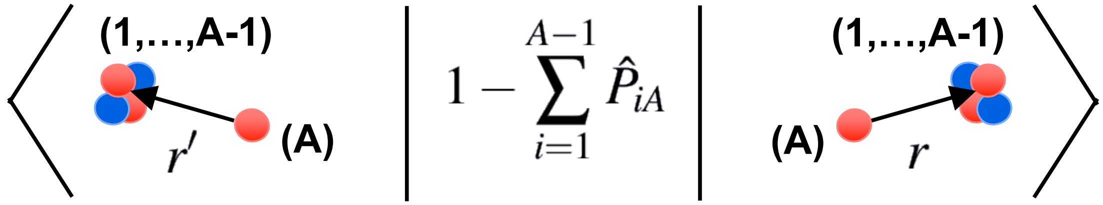
$$[\hat{T}_{\mathrm{rel}}(r) + \bar{V}_{\mathrm{C}}(r) - (E - E_\nu)]\, u_\nu(r) + \sum_{\nu} \int dr'\, r'\, W_{\nu\nu'}(r, r')\, u_\nu(r') = 0$$



Fully implemented and tested for single-nucleon projectile (nucleon-nucleus) basis

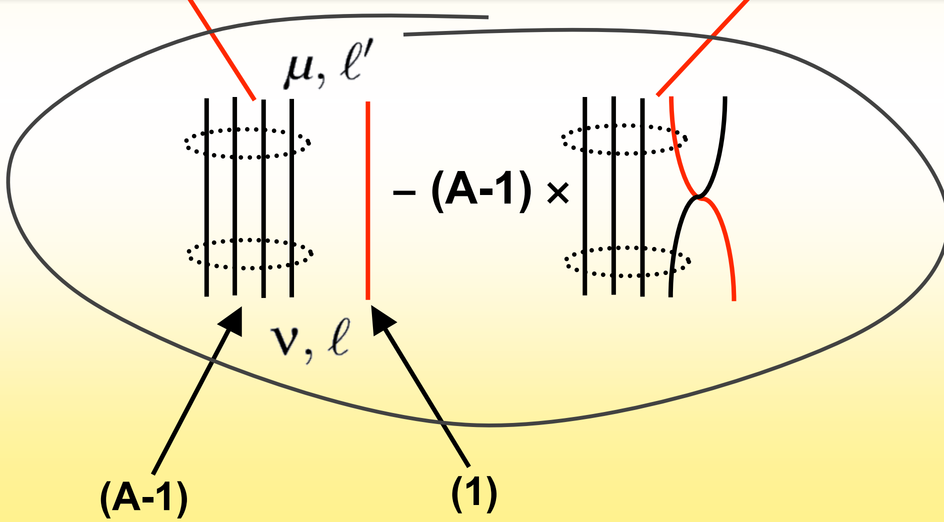
Single-nucleon projectile: the norm kernel



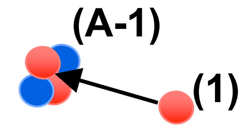


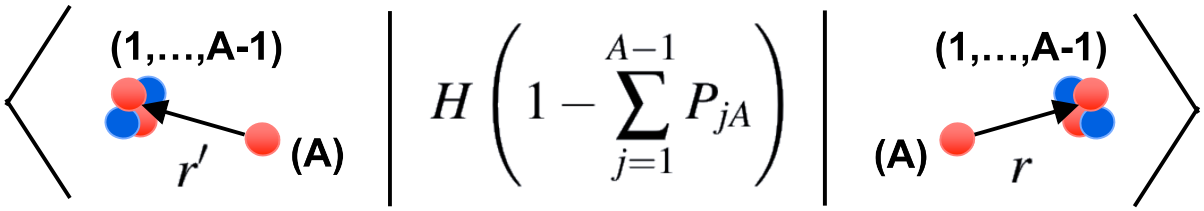
$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

$${}_{SD}\langle\psi^{(A-1)}_{\mu_1}|a^+a|\psi^{(A-1)}_{\nu_1}\rangle_{SD}$$



Single-nucleon projectile basis: the Hamiltonian kernel





$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r,r') = [\hat{T}_{\rm rel}(r') + \bar{V}_{\rm Coul}(r') + E_\mu]\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

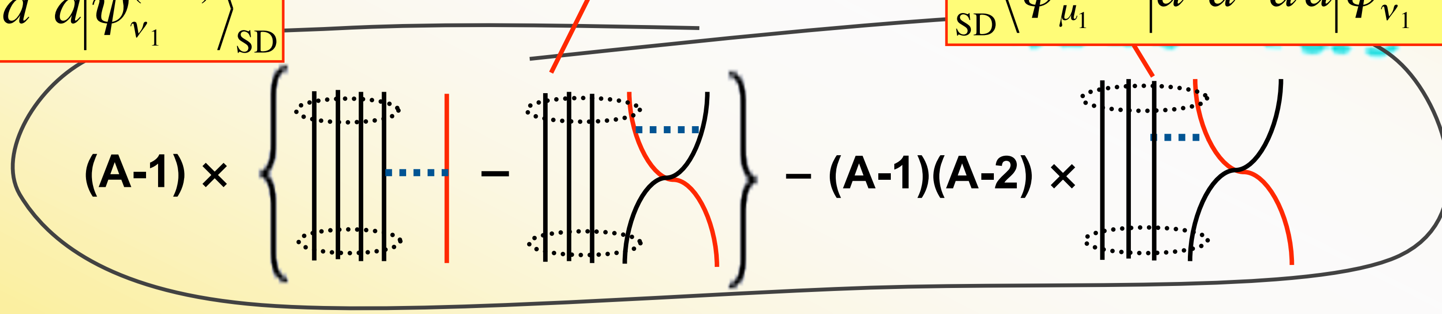
$$+ (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|V_{A-1,A}(1-P_{A-1,A})|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

$$-(A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|V_{A-2,A}P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

+ terms containing NNN potential

$${}_{\rm SD}\left\langle\psi^{(A-1)}_{\mu_1}\right|a^+a\left|\psi^{(A-1)}_{\nu_1}\right\rangle_{\rm SD}$$

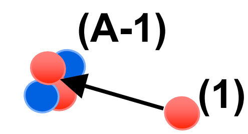
$${}_{\rm SD}\left\langle\psi^{(A-1)}_{\mu_1}\right|a^+a^+\,a\,a\left|\psi^{(A-1)}_{\nu_1}\right\rangle_{\rm SD}$$



"direct potential"

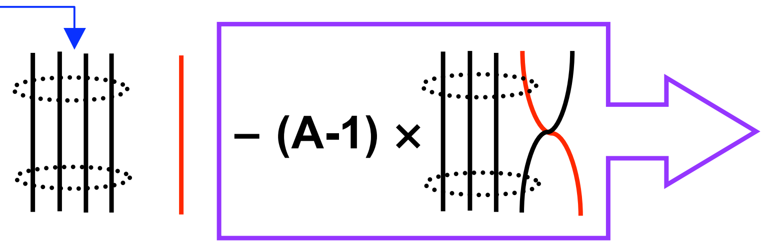
"exchange potential"

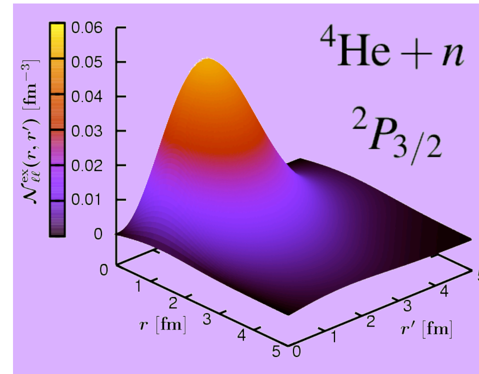
The RGM kernels in the single-nucleon projectile basis



$$\delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r}$$

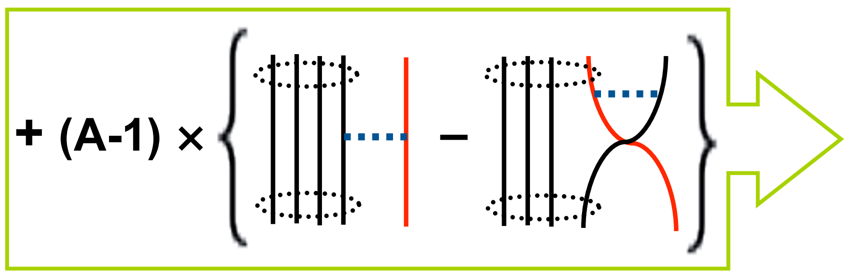
$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) =$$

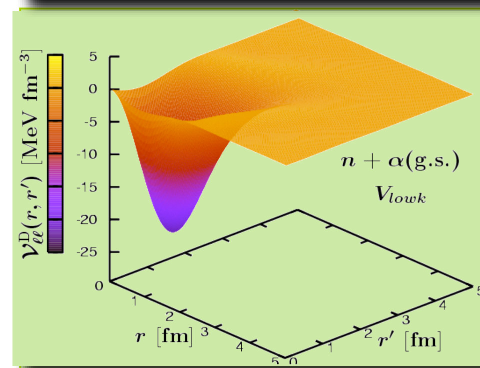


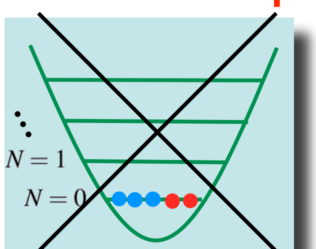


$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r,r') = [\hat{T}_{\rm rel}(r') + \bar{V}_{\rm Coul}(r') + E_\mu]\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

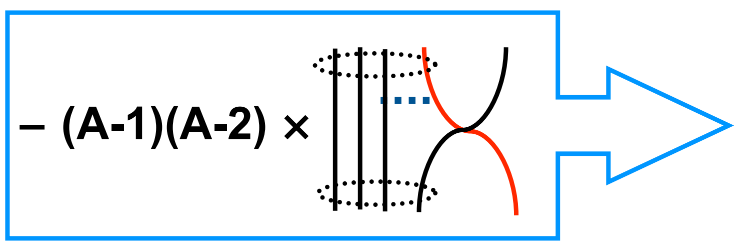
"direct potential"

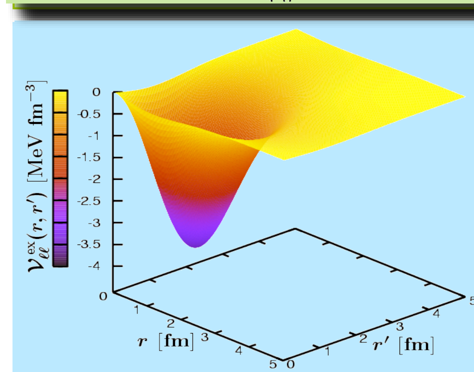




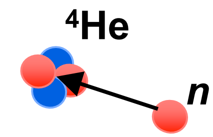


"exchange potential"

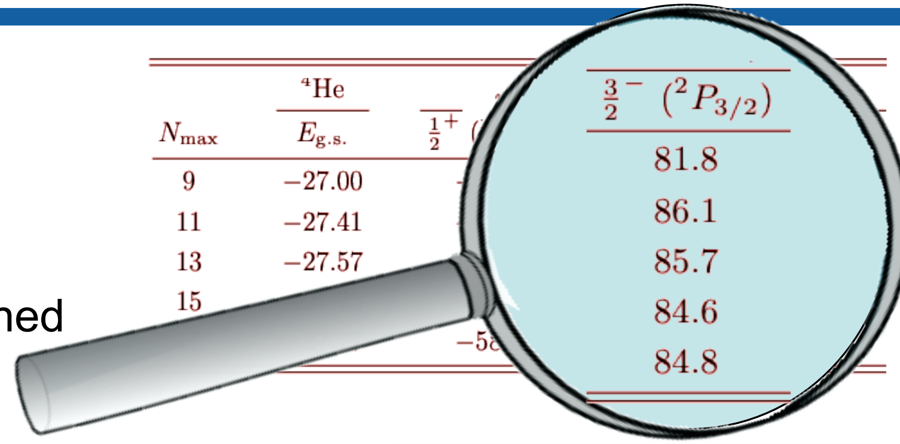




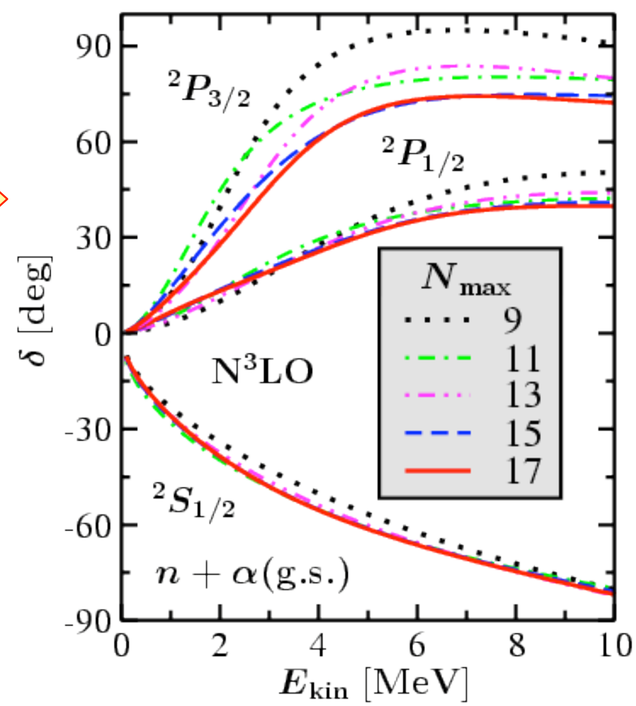
NCSM/RGM *ab initio* calculation of *n*-^{4}He phase shifts

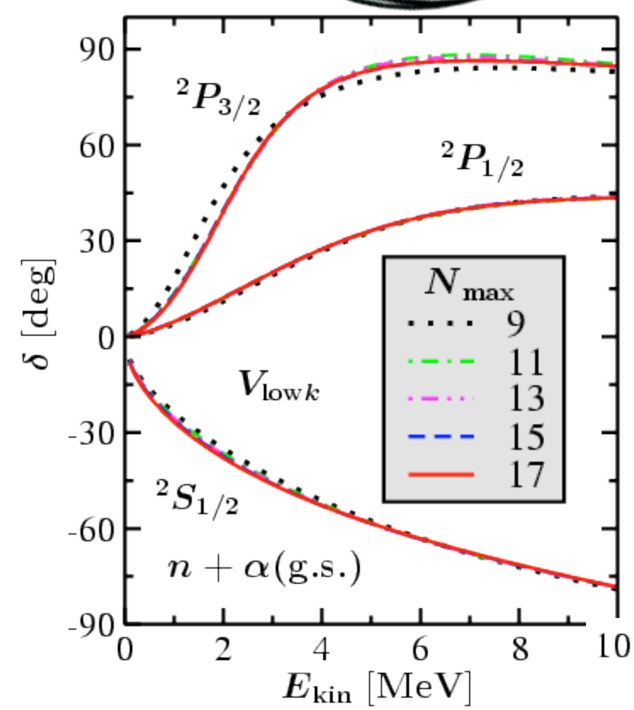


- NCSM/RGM calculations with *n*+^{4}H(g.s.)
- Low-momentum V_{lowk} NN potential: convergence reached with bare interaction
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction



Fully *ab initio*. No fit.
No free parameters.
Convergence in N_{max} under control.

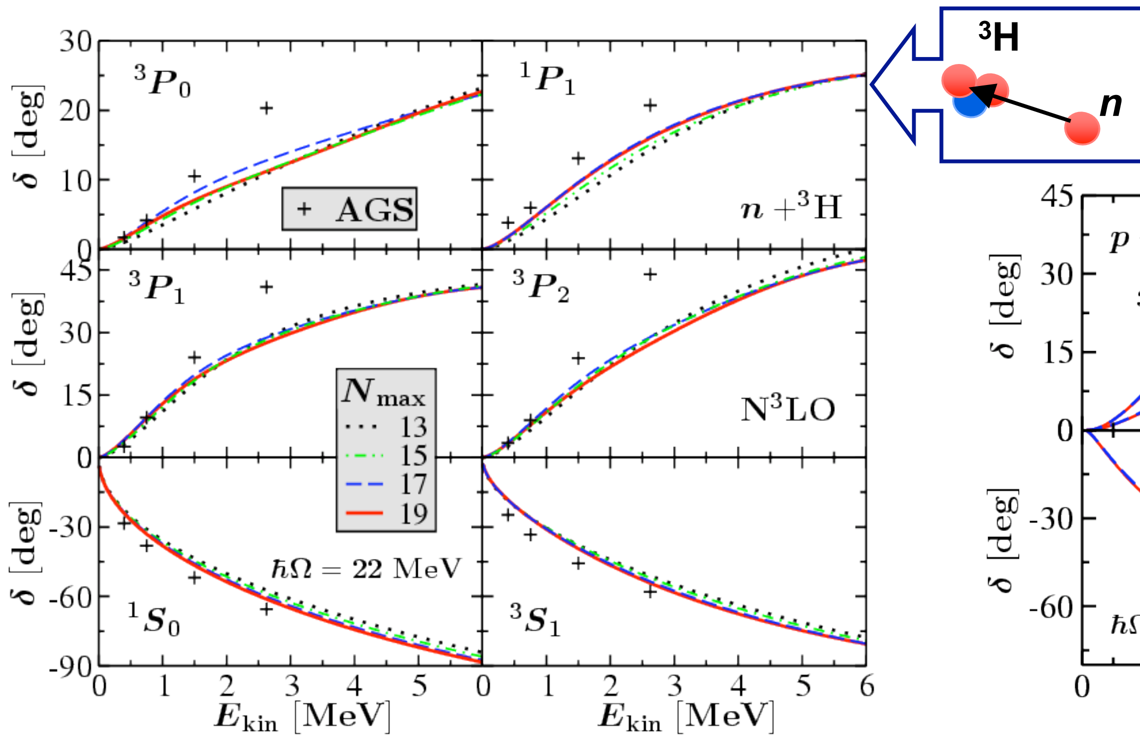


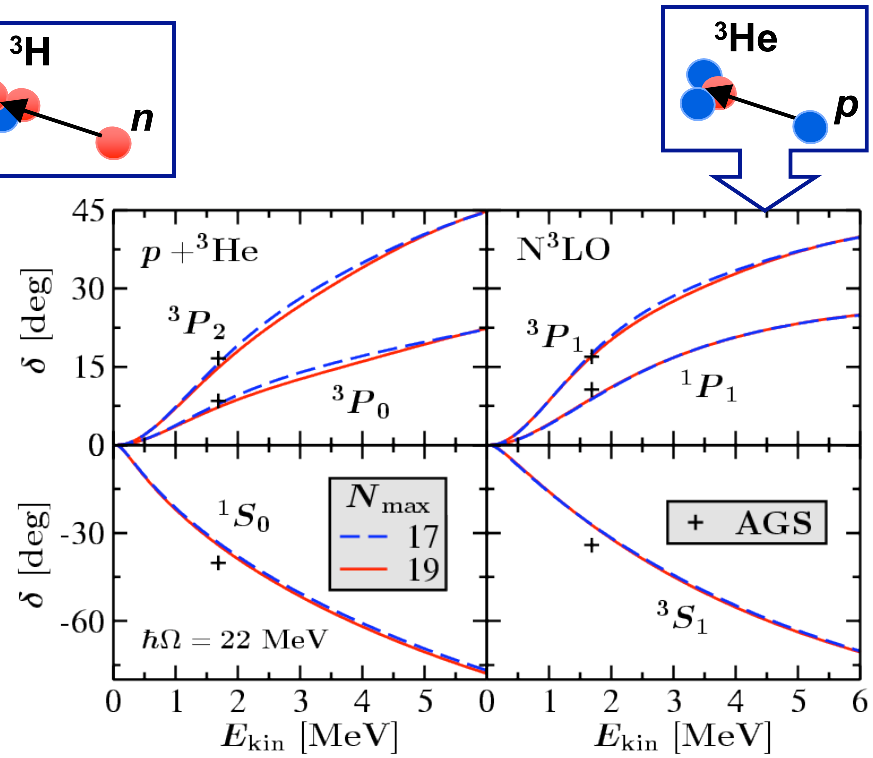


Is everything else under control? … need verification against independent *ab initio* approach!

NCSM/RGM *ab initio* calculation of n-^{3}H and p-^{3}He phase shifts

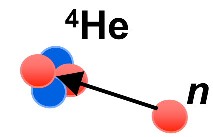
- NCSM/RGM calculations with n+^{3}H(g.s.) and p+^{3}He(g.s.), respectively.
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction
- Benchmark with Alt, Grassberger and Sandhas (AGS) results [**PRC75, 014005(2007)**]
  - What is missing? - n+^{3}H(ex), ^2n+d, p-^{3}He(ex), ^{2}p+d configurations



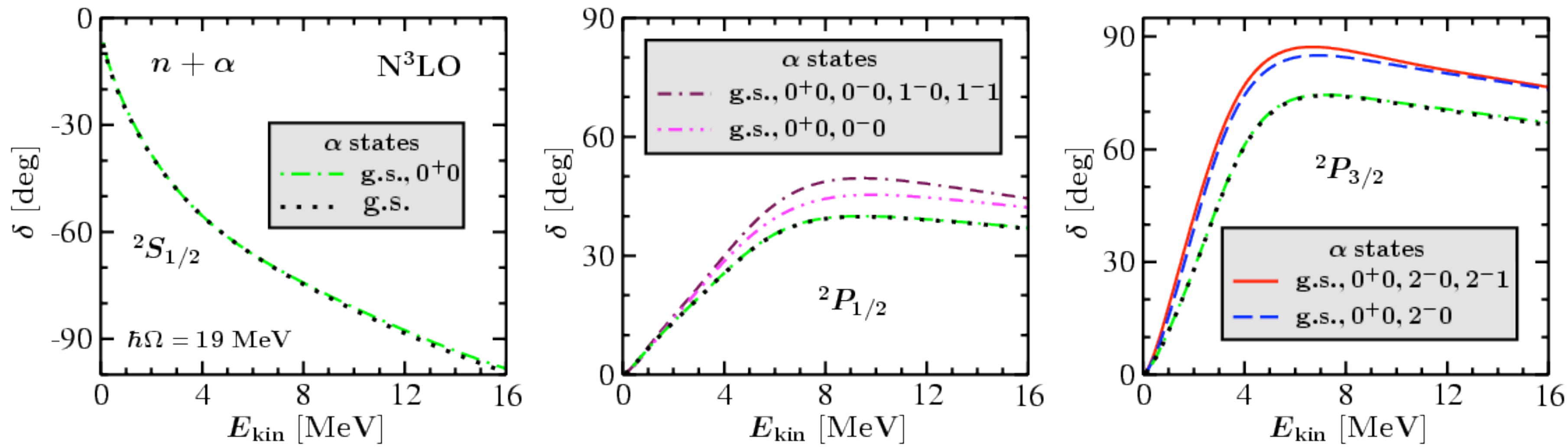


The omission of three-nucleon partial waves with $1/2 < J \leq 5/2$ leads to effects of comparable magnitude on the AGS results. Need to include target excited states!

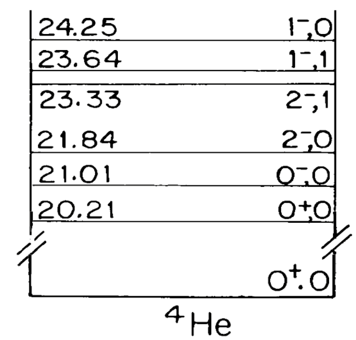
n-^{4}He phase shifts with χEFT N^{3}LO NN interaction



- NCSM/RGM calculation with n+^{4}He(ex)
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction



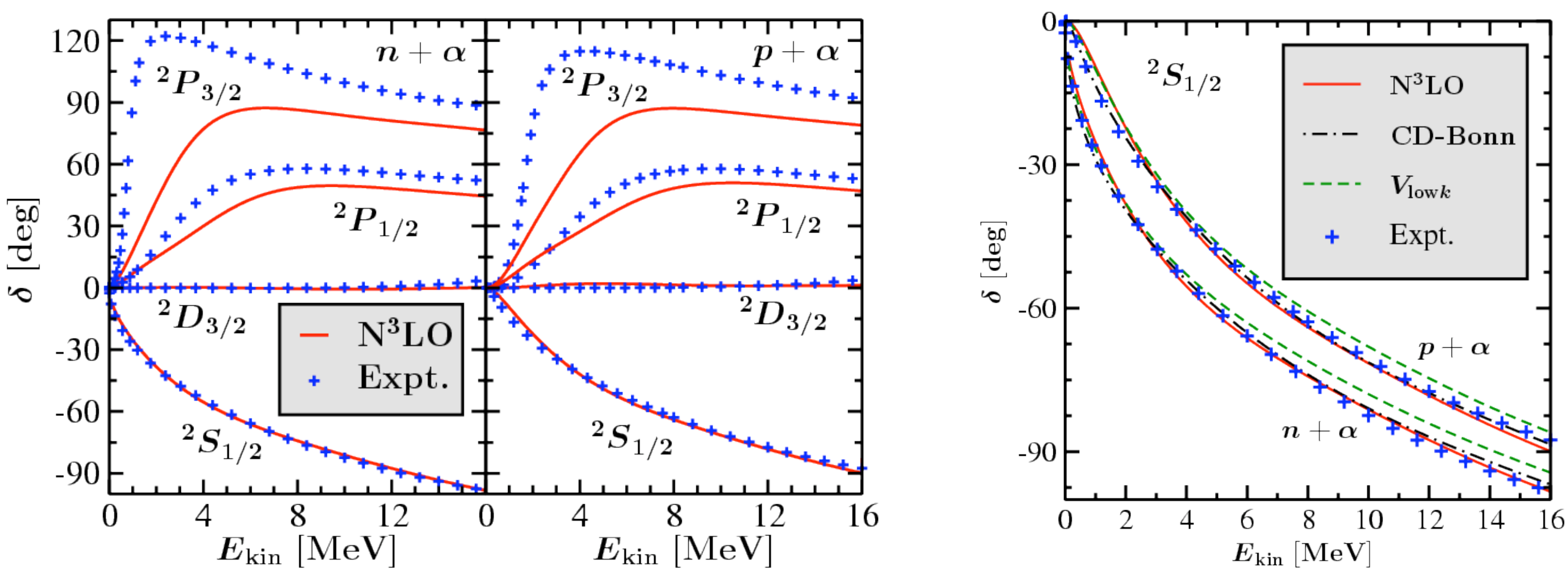
- very mild effects of 0^+0 on $^2S_{1/2}$
- the negative-parity states have larger effects on $^2P_{1/2}$ and $^2P_{3/2}$
  - 0^-0, 1^-0 and 1^-1 affect $^2P_{1/2}$
  - 2^-0 and 2^-1 affect $^2P_{3/2}$



The resonances are sensitive to the inclusion of the first six excited states of ^{4}He.

Nucleon-α phase-shifts with χEFT N^{3}LO NN interaction

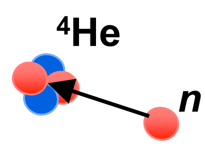
- NCSM/RGM calculation with N+^{4}He(g.s., 0^+0, 0^-0, 1, 1^-0, 2^-0, 2^-1)
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction
- $^2S_{1/2}$ in agreement with Expt. (dominated by N-α repulsion induced by Pauli principle)
- Insufficient spin-orbit splitting between $^2P_{1/2}$ and $^2P_{3/2}$ (sensitive to interaction model)



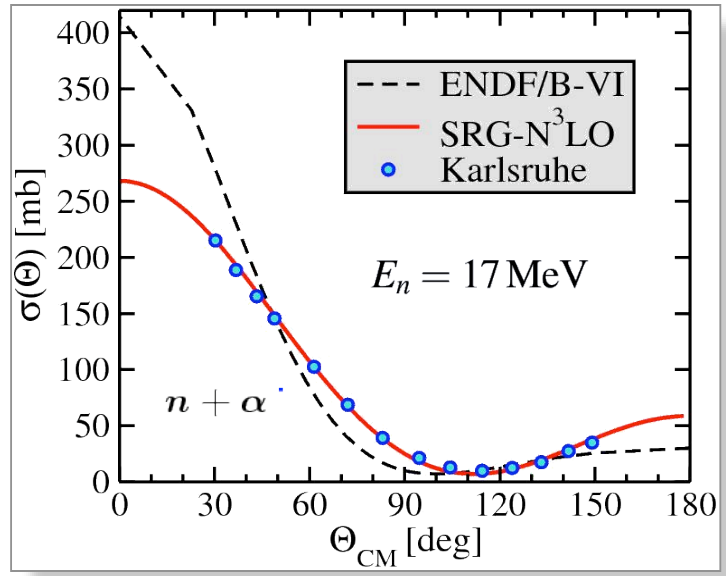
The first n-^{4}He and p-^{4}He phase shifts calculation within the NCSM/RGM approach.
Fully *ab initio*, very promising results. The resonances are sensitive to NNN interaction.

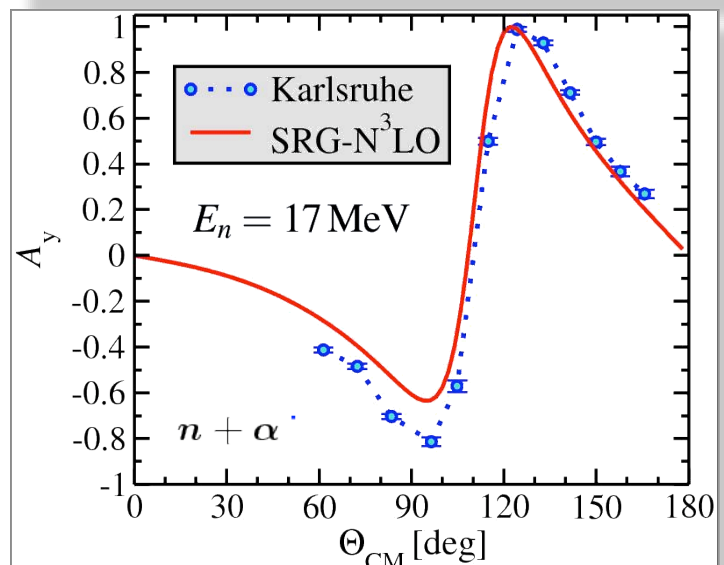
n+^{4}He differential cross section and analyzing power

- Neutron energy of 17 MeV
  - beyond low-lying resonances
- Polarized neutron experiment at Karlsruhe
- NCSM/RGM calculations
  - n+^{4}He(g.s,0+0)
  - SRG-evolved N^{3}LO NN potential



- Good agreement for angular distribution
- Differences for analyzing power
  - A_y puzzle for A=5?

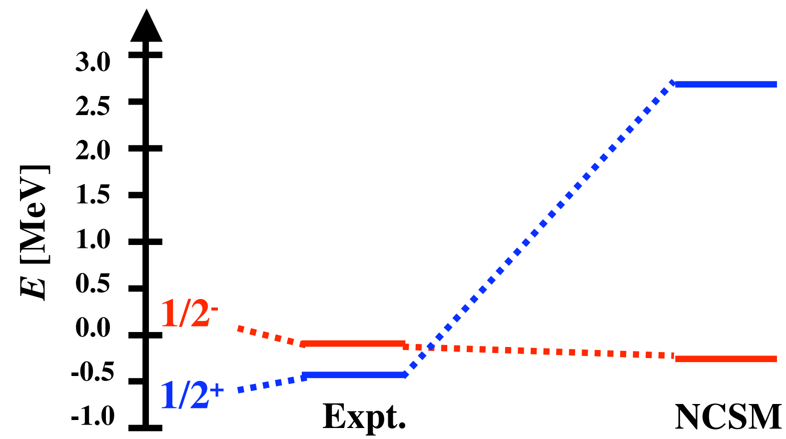




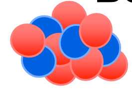
First ever *ab initio* calculation of A_y in for a A=5 system. Strict test of inter-nucleon interactions.

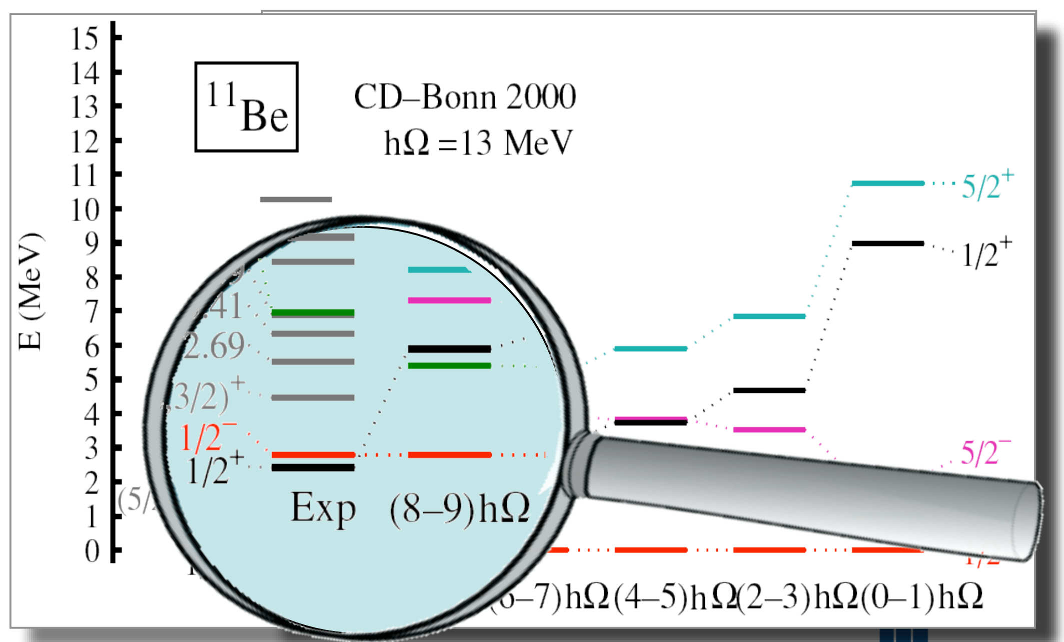
^{11}Be bound states and *n*-^{10}Be phase shifts

- ^{11}Be: 1/2^{+} g.s. instead of *p*-shell expected 1/2^{-}
  - disappearance of *N*=8 magic number with increasing *N/Z* ratio
- Large-scale *ab initio* NCSM calculations from Forssen *et al.* Phys. Rev. C **71**, 044312 (2005)
  - several realistic NN potentials
  - do not explain parity inversion



^{11}Be

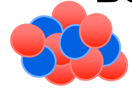




^{11}Be bound states and *n*-^{10}Be phase shifts

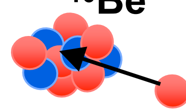
- ^{11}Be: 1/2$^+$ g.s. instead of *p*-shell expected 1/2$^-$
  - disappearance of *N*=8 magic number with increasing *N/Z* ratio
- Large-scale *ab initio* NCSM calculations from Forssen *et al.* Phys. Rev. C **71**, 044312 (2005)
  - several realistic NN potentials
  - do not explain parity inversion

^{11}Be

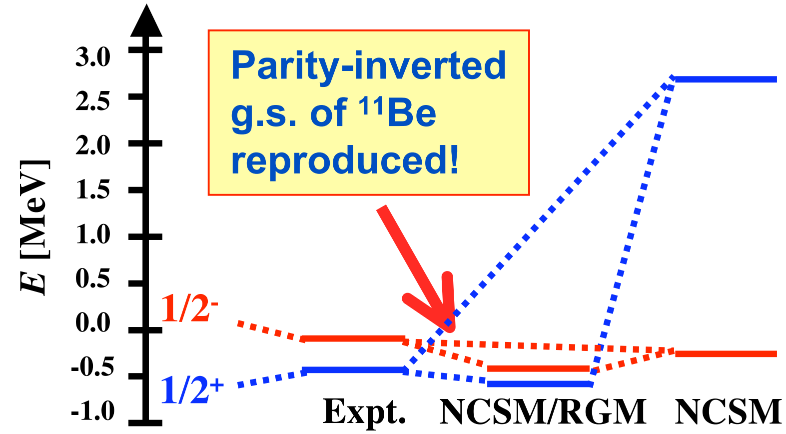


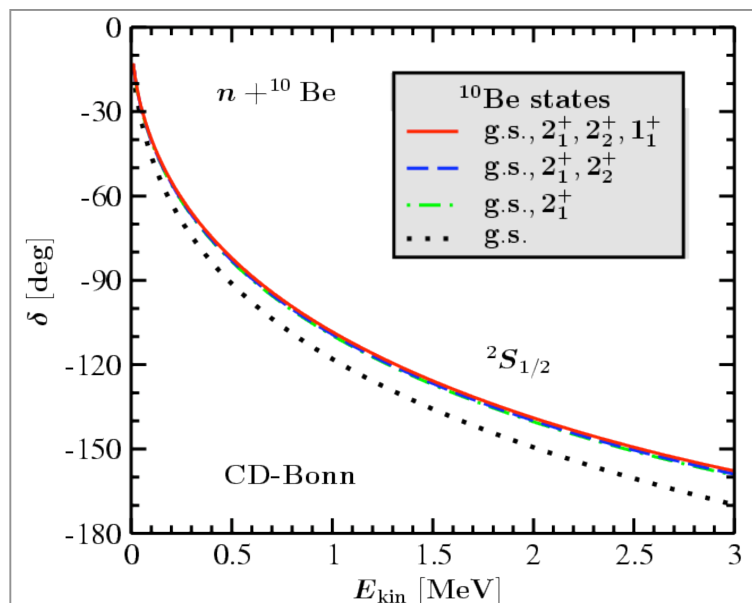
- NCSM/RGM calculations from S.Q. and P. Navratil, Phys. Rev. Lett. **101**, 092501 (2008)
  - n+^{10}Be(g.s.,2_1^+,2_2^+,1_1^+)
  - realistic CD-Bonn NN potential
  - reproduce parity inversion

^{10}Be

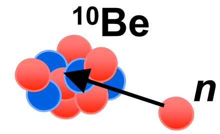


	$N_{\max}$	^{10}Be $E_{\rm g.s.}$	^{11}Be($\frac{1}{2}^-$) E	^{11}Be($\frac{1}{2}^-$) E_{th}	^{11}Be($\frac{1}{2}^+$) E	^{11}Be($\frac{1}{2}^+$) E_{th}
NCSM	8/9	-57.06	-56.95	0.11	-54.26	2.80
NCSM	6/7	-57.17	-57.51	-0.34	-54.39	2.78
NCSM/RGM			-57.59	-0.42	-57.85	-0.68
Expt.		-64.98	-65.16	-0.18	-65.48	-0.50

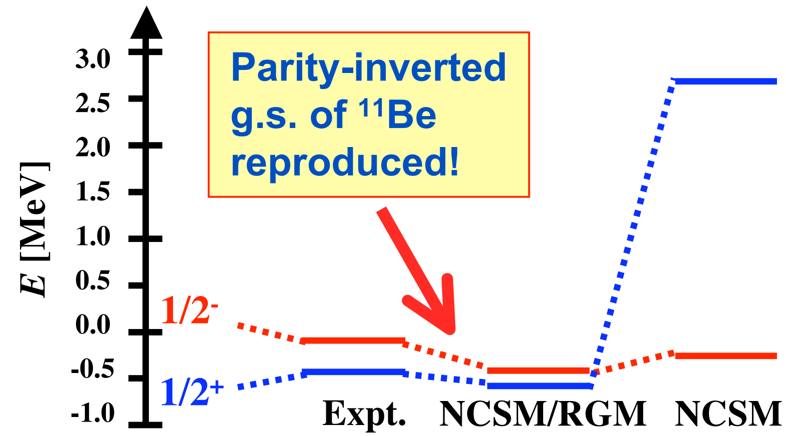




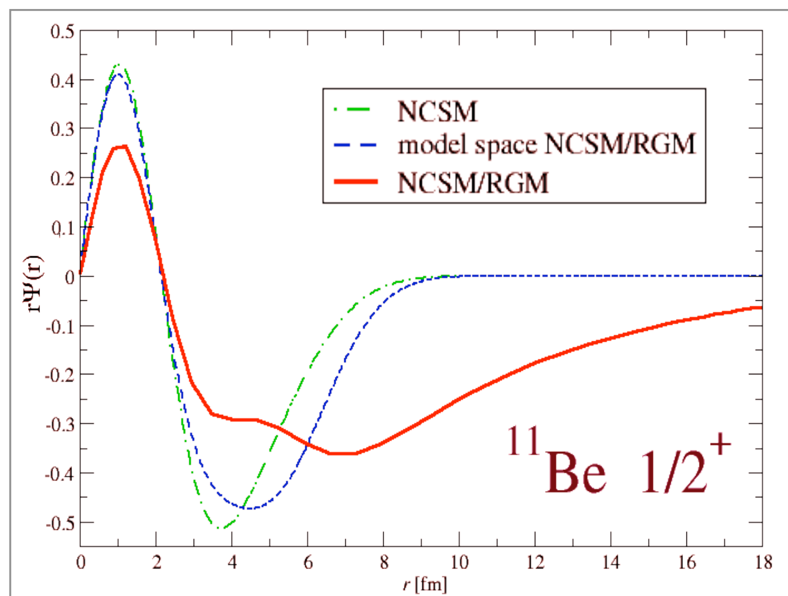
^{11}Be bound states and *n*-^{10}Be phase shifts



- What happens?
  - The *n*-^{10}Be w.f. has a large extension
  - When the Whittaker tail is recovered, the w.f. internal region is rescaled
  - Relative kinetic and potential energies decrease in absolute value
    - kinetic energy more dramatically
  - Net effect: gain in binding energy



NCSM/RGM	$\langle T_{rel} \rangle$	$\langle W \rangle$	$E[^{10}\text{Be(g.s., ex.)}]$	E_{tot}
Model Space	16.65	−15.02	−56.66	−55.03
Full	6.56	−7.39	−57.02	−57.85

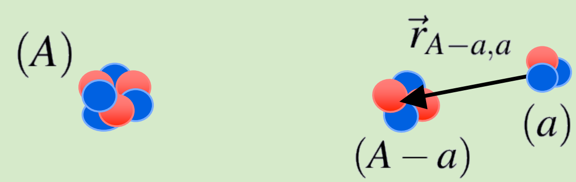


Only when an approach is capable of describing the ^{11}Be halo can one obtain a meaningful insight on the parity-inversion of its ground state.

Conclusions and outlook

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
- Our recent results in PRL 101, 092501 (2008); PRC (2009) in print, arXiv:0901.0950
  - *n*-^{3}H, *n*-^{4}He, *n*-^{10}Be and *p*-^{3,4}He scattering phase-shifts with realistic NN potentials
  - study of the parity-inverted ground state of ^{11}Be
- More work ahead!
  - Inclusion of NNN force
  - Binary cluster basis with d, ^{3}H,^{3}He,^{4}He projectiles
  - Need three-body cluster basis
    - three-body breakup
    - two-nucleon halos
  - New model space spanned by NCSM + NCSM/RGM bases

  ➔ NCSM with continuum (NCSMC)



$$\left|\Psi_A^J\right\rangle = \sum c_\lambda \left|A\lambda J\right\rangle + \sum \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi_{\nu\vec{r}}^{(A-a,a)}$$

$$\begin{pmatrix} H & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix} = E \begin{pmatrix} 1 & g \\ g & \mathcal{N} \end{pmatrix} \begin{pmatrix} c \\ \varphi \end{pmatrix}$$