Lawrence Livermore National Laboratory

Ab initio many-body calculations of nucleon-nucleus scattering

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UNEDF SCIDAC meeting, Pack Forest, WA,6/26/2008

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

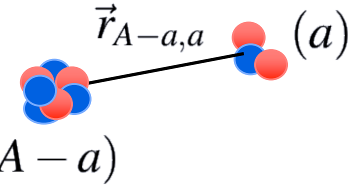
LLNL-PRES-404833

Ab initio approach to light-ion reactions

- Combining the *ab initio* no-core shell model (NCSM)

  with the resonating group method (RGM)

  $\Rightarrow$ ***ab initio* NCSM/RGM**
  - NCSM - single-particle degrees of freedom
  - RGM - clusters and their relative motion



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

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

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

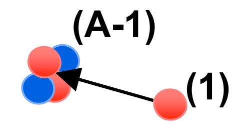
Norm kernel: $\langle\Phi^{(A-a,a)}_{\mu\vec{r}\,'}|\hat{\mathcal{A}}^2|\Phi^{(A-a,a)}_{\nu\vec{r}}\rangle$

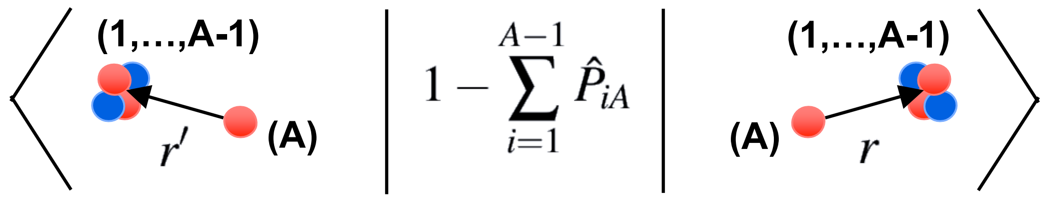
- Non-local integro-differential coupled-channel equations:

$$[T_c + \bar{V}_C(r) - (E-\varepsilon_c)]u_c(r) + \sum_{c'}\int dr'\,r'^2 W_{cc'}(r,r')u_{c'}(r') = 0$$

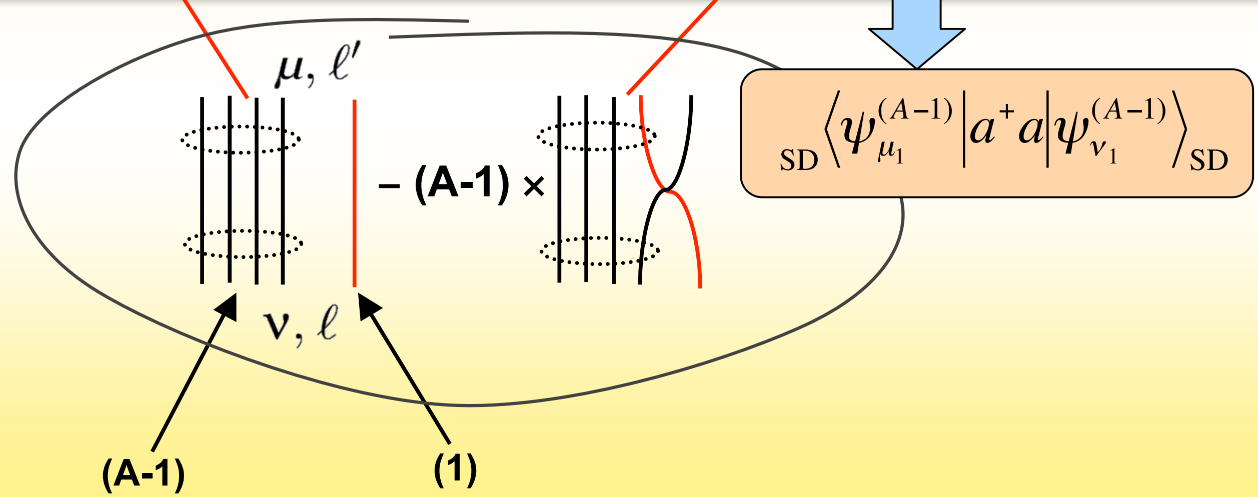
Fully implemented and tested for the case of a single-nucleon projectile (nucleon-nucleus system). Capability to calculate bound states, scattering matrix, phase shifts, cross sections.

Single-nucleon projectile: the norm kernel

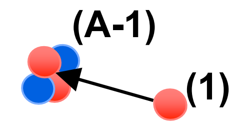


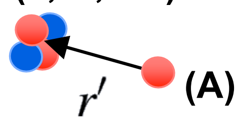


$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)=\delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r}-(A-1)\sum_{n'n}R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

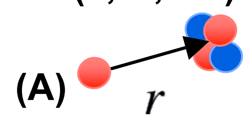


Single-nucleon projectile basis: the Hamiltonian kernel





$$H\left(1-\sum_{j=1}^{A-1} P_{jA}\right)$$



$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = (E_{A-1}+\mathcal{T}_{rel})\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

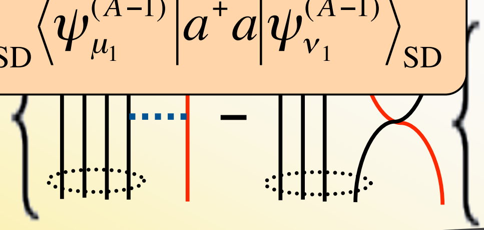
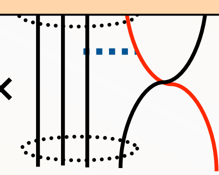
$$+\,(A-1)\sum_{n'n} R_{n'\ell'}(r')\,\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|V_{A-1,A}(1-P_{A-1,A})|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle\, R_{n\ell}(r)$$

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

\+ terms containing 3N potential

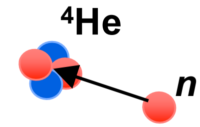
$${}_{SD}\langle\psi^{(A-1)}_{\mu_1}|a^+a|\psi^{(A-1)}_{\nu_1}\rangle_{SD}$$

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

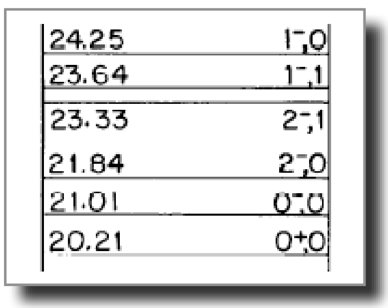
(A-1) ×  **– (A-1)(A-2) ×** 

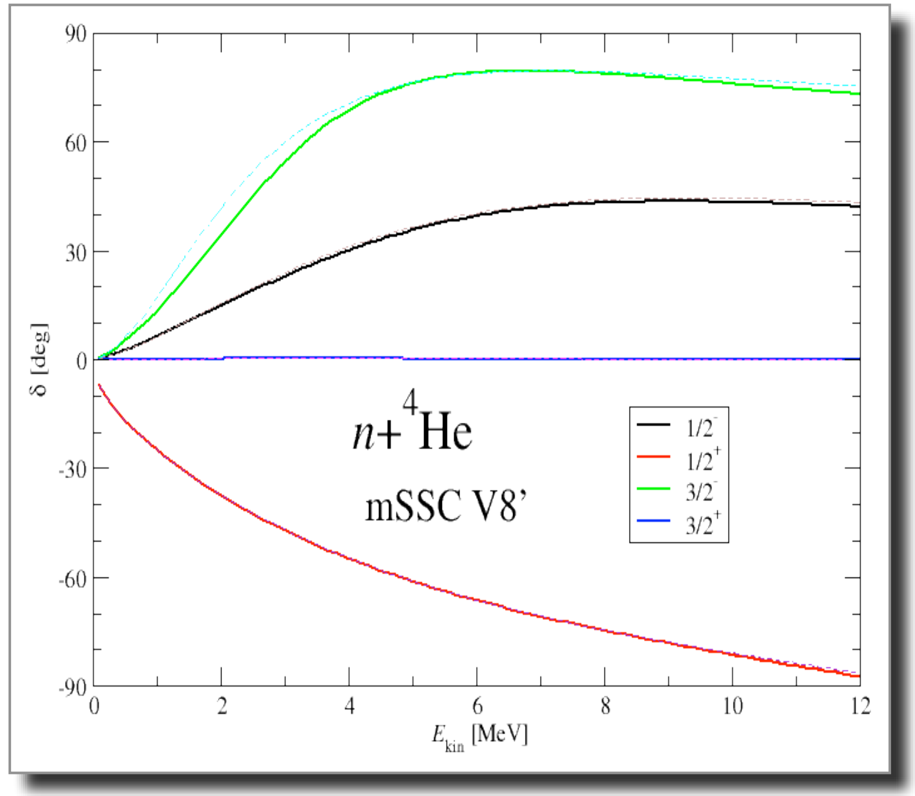
"direct potential" "exchange potential"

n-^{4}He phase shifts with mSSC V8' NN interaction



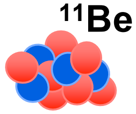
- NCSM/RGM calculation:
  - mSSC V8' NN potential
  - two-body effective interaction N_{max}=17 @ $\hbar\Omega$ = 22 MeV
    - Dotted lines N_{max}=15
  - ^{4}He states: g.s. + 0^+0
- p+^{4}He calculated as well



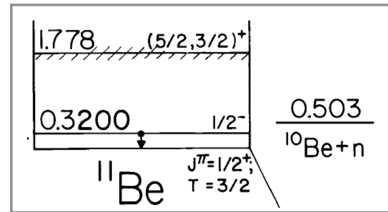


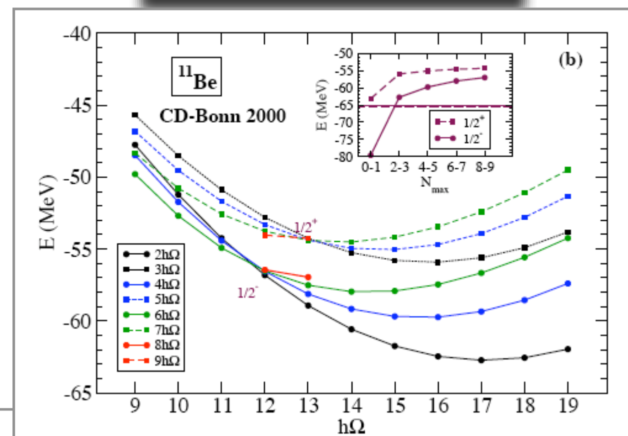
Done with the NN potential used for UNEDF benchmarks. Other resonances still should be included: 0^- 0, 1^- 0, 2^- 0. To be compared to GFMC calculations.

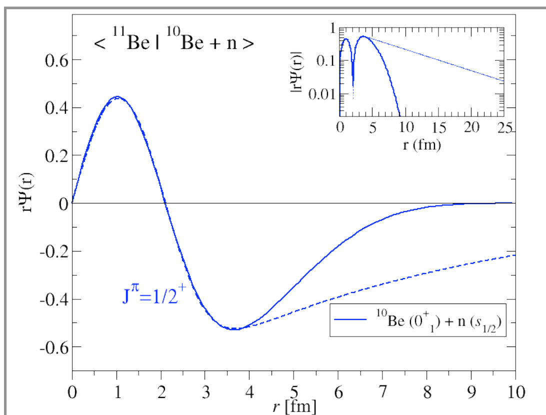
Parity-inverted ground state of ^{11}Be

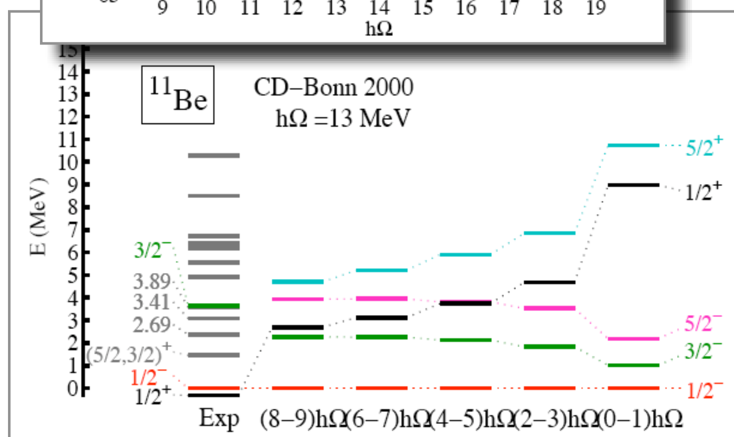


- **^{11}Be**
  - Disappearance of *N*=8 magic number with increasing *N/Z* ratio
  - Ground state $1/2^+$ instead of the *p*-shell expected $1/2^-$
- Large-scale *ab initio* NCSM calculations with several accurate NN potentials do not explain the parity inversion
  - PRC **71**, 043312 (2005)
- Problem:
  - Extended n+^{10}Be configurations suppressed

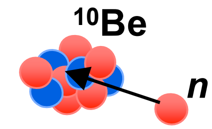






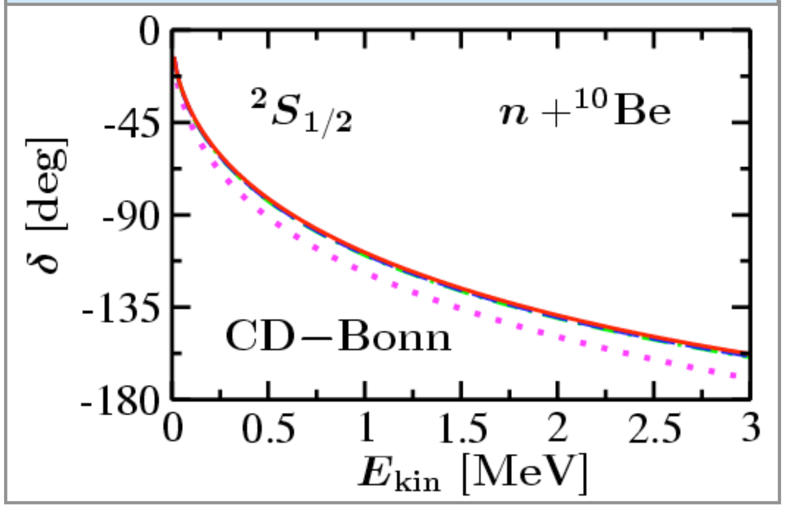


n-^{10}Be phase shifts with CD-Bonn NN interaction



- NCSM/RGM calculation:
  - CD-Bonn 2000 NN potential
  - two-body effective interaction
    N_{max}=7 @ $\hbar\Omega$ = 13 MeV
  - ^{10}Be states:
    - (solid red) g.s., 2_1^+, 2_2^+, 1_1^+
    - (blue dashed) g.s., 2_1^+, 2_2^+
    - (green dash-dot) g.s., 2_1^+
    - (magenta dotted) g.s.

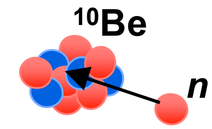
n-^{10}Be phase shifts



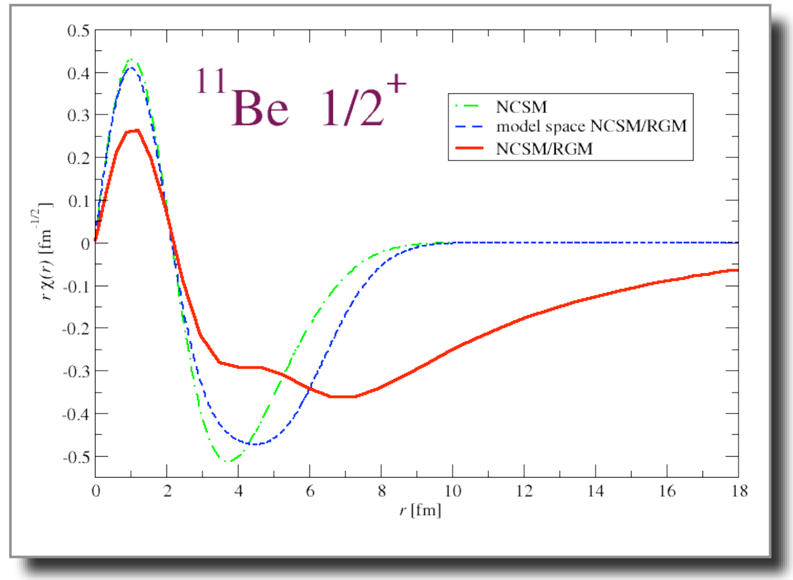
	$N_{\max}$	^{10}Be $E_{g.s.}$	^{11}Be($\frac{1}{2}^-$) E	^{11}Be($\frac{1}{2}^-$) E_{th}	^{11}Be($\frac{1}{2}^+$) E	^{11}Be($\frac{1}{2}^+$) E_{th}
NCSM	8/9	-57.06	-56.95	0.11	-54.26	2.80
NCSM	6/7	-57.17	-57.51	-0.34	-54.39	2.78
RGM/NCSM			-57.59	-0.42	-57.85	-0.68
Expt.		-64.98	-65.16	-0.18	-65.48	-0.50

- Dramatic increase of ^{11}Be $1/2^+$ binding energy
- Inversion between $1/2^-$ and $1/2^+$ states reproduced

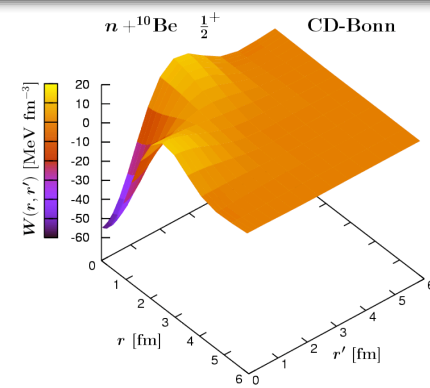
n-^{10}Be & parity-inverted ground state of ^{11}Be



- What happens?
  - *n*-^{10}Be wave function extends to large distances
  - Relative kinetic and potential energies decrease in absolute values
  - The kinetic energy more dramatically
    - Net effect: **Gain in binding energy**

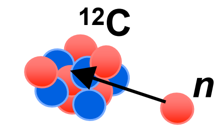


NCSM /RGM	T_{rel}	V_{rel}	E_{10Be}	E_{tot}
Model-space	16.65	-15.02	-56.66	-55.03
Full	6.56	-7.39	-57.02	-57.85

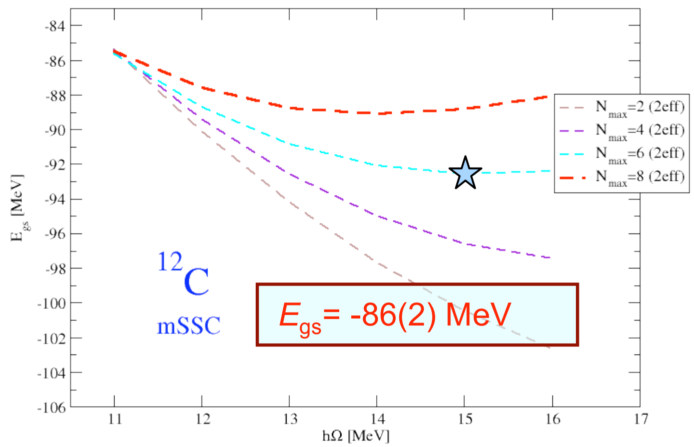


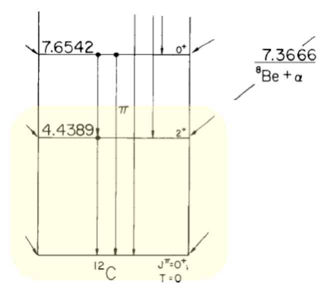
The proper description of extended *n*-^{10}Be configurations leads to parity-inverted ^{11}Be g.s.

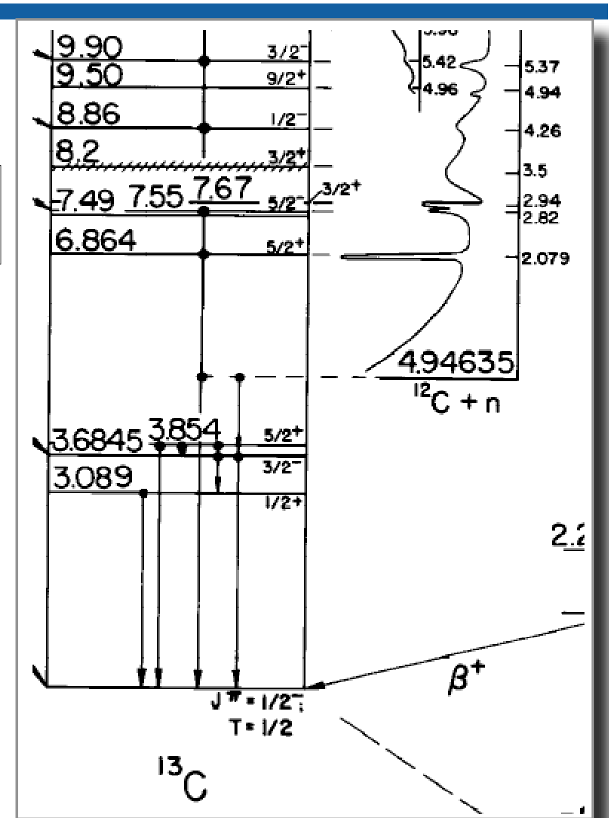
n-^{12}C scattering with mSSC V8' NN interaction

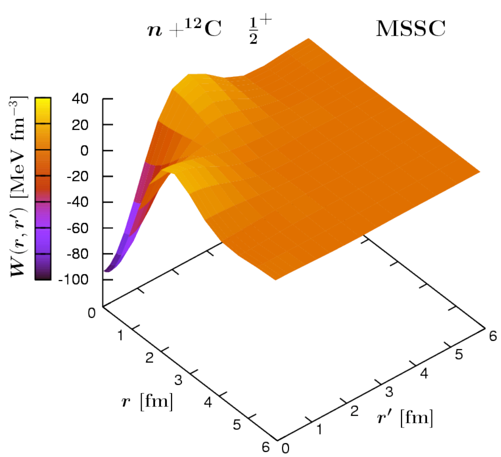


- NCSM ^{12}C benchmark calculation: E_{gs}=-86(2) MeV
- NCSM ^{13}C calculation:
  - 1/2⁺, 5/2⁺ states too high, unbound
- NCSM/RGM ^{13}C calculation:
  - two-body effective interaction N_{max}=7 @ $\hbar\Omega$ = 14 MeV
  - ^{12}C states: g.s., 2^+_1
    - 1/2⁺ state bound
    - 1/2⁻, 3/2⁻ and 5/2⁺ bound



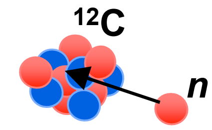






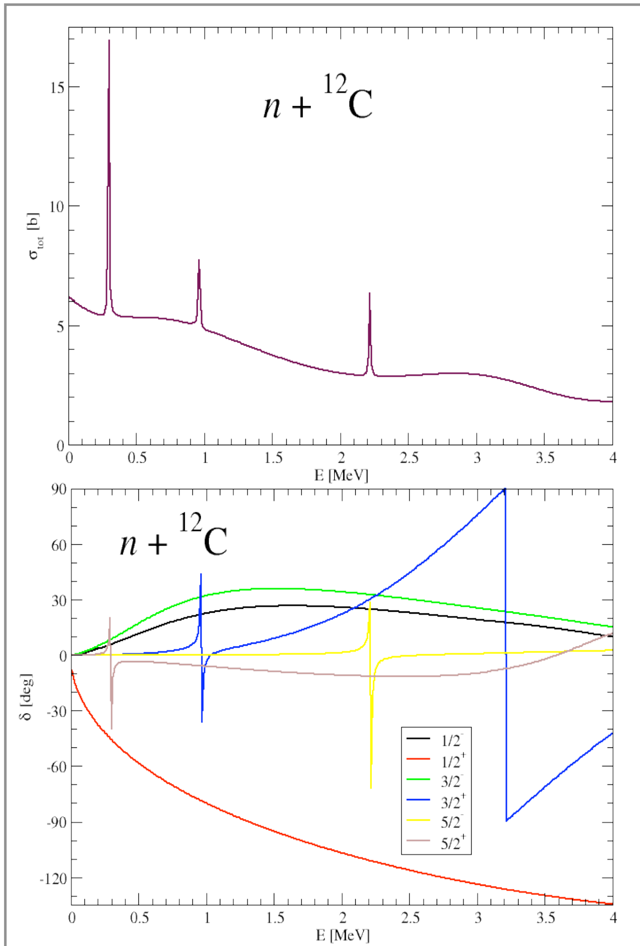
	^{12}C	^{13}C: $\frac{1}{2}^-$		$\frac{3}{2}^-$	$\frac{1}{2}^+$	$\frac{5}{2}^+$
	$E_{g.s.}$	$E_{g.s.}$	E_{th}		E_{th}	
NCSM $6\hbar\Omega/7\hbar\Omega$	-92.59	-101.18	-8.59	-7.11	+0.08	+1.49
NCSM/RGM		-99.72	-7.13	-5.35	-2.85	-0.62
Expt.	-92.16	-97.11	-4.95	-1.26	-1.86	-1.09

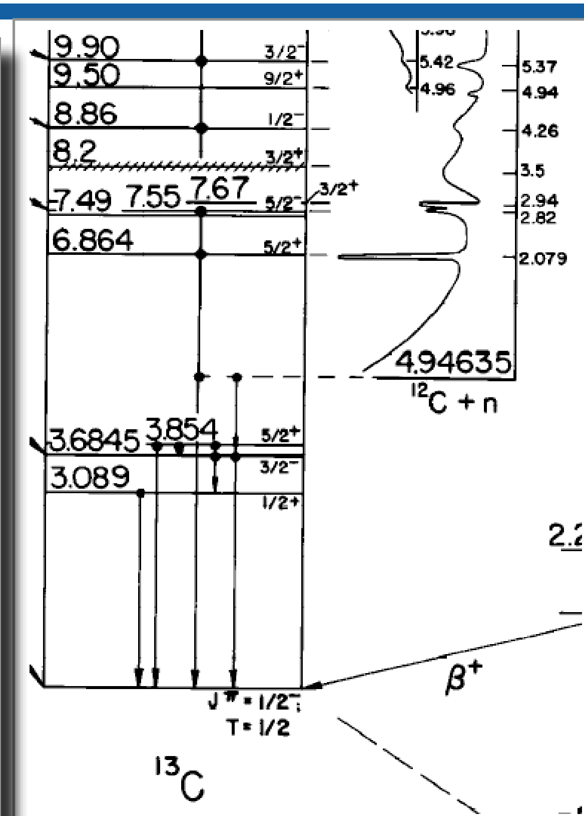
n-^{12}C scattering with mSSC V8' NN interaction



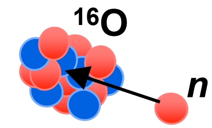
- NCSM/RGM *n*+^{12}C total cross section dominated by *d*-wave resonances
  - $5/2^+$, $3/2^+$ states in ^{13}C
  - $1/2^-$, $3/2^-$, 1/2+ and $5/2^+$ states bound
  - $5/2^+$, $3/2^+$ and $5/2^-$ narrow resonances
  - $3/2^+$ broad resonance

- Scattering calculation a much stricter test of NN (+NNN) interactions than the discrete state calculation alone

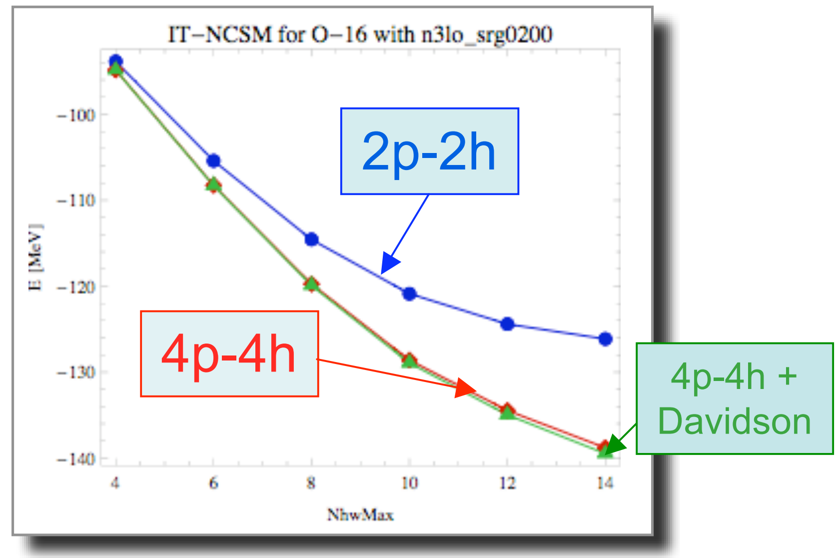




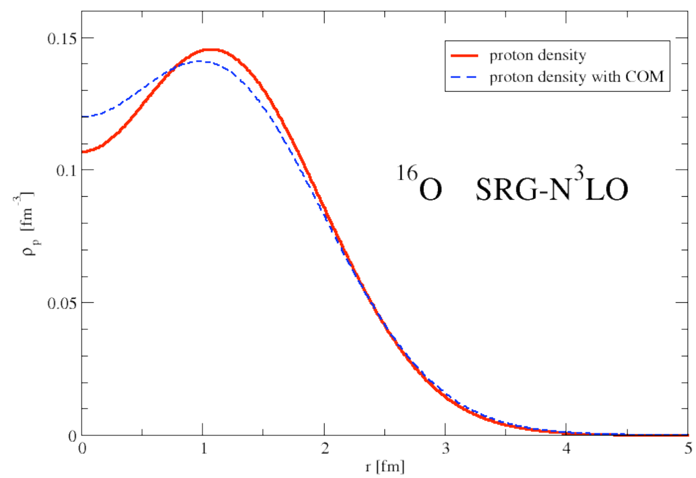
n-^{16}O scattering with SRG-N^{3}LO NN potential



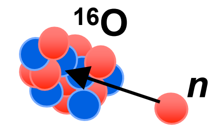
- ^{16}O ground state calculated within importance-truncated NCSM
  - in collaboration with R. Roth (TU Darmstadt)
  - 4p-4h up to N_{max}=14 (N_{max}=18 possible!?), $h\Omega$=20 MeV
  - SRG-N^{3}LO with Λ=2.66 fm^{-1}
    - Less overbinding
  - Benchmarking with full NCSM
    - ^{16}O binding energy up to N_{max}=8
    - **Perfect agreement**



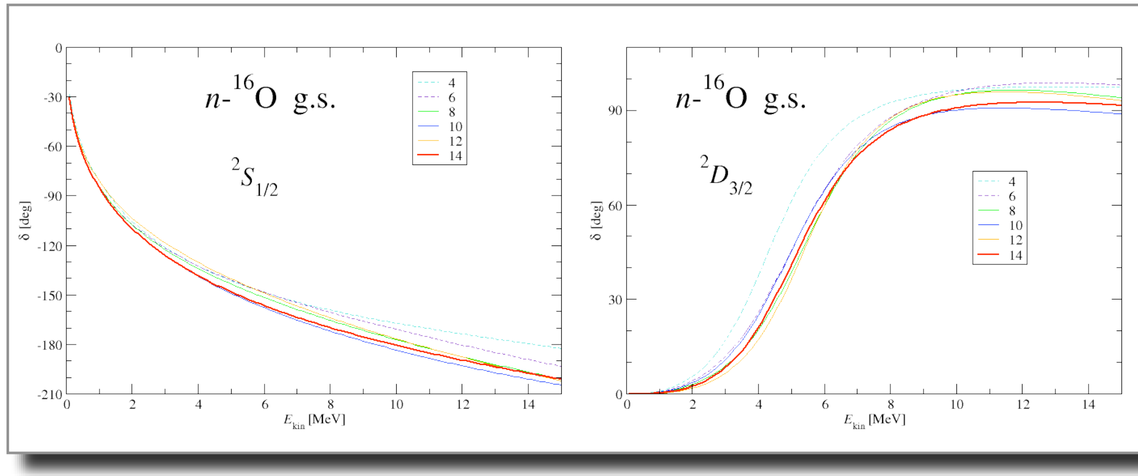
- ^{17}O within *ab initio* NCSM/RGM
  - 1/2$^+$ bound: E_b=-0.87 MeV wrt ^{16}O
  - 5/2$^+$ bound: E_b=-0.40 MeV wrt ^{16}O
    - N_{max}=15, $h\Omega$=20 MeV
    - Only ^{16}O ground-state included

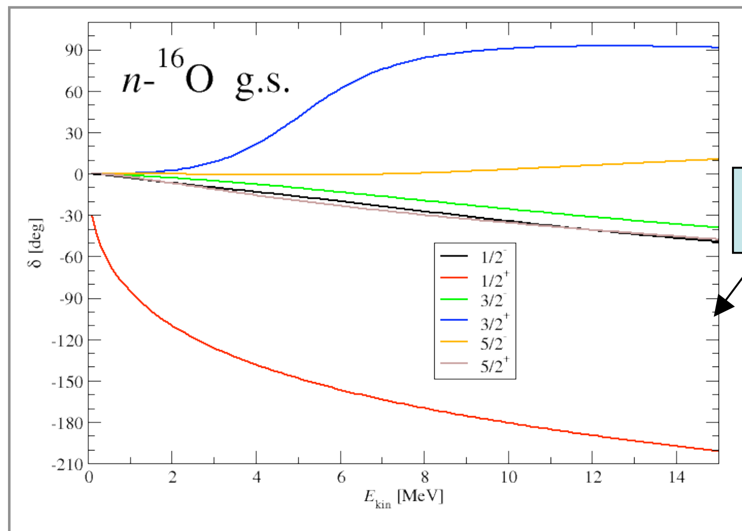


n-^{16}O scattering with SRG-N^{3}LO NN potential



- Phase-shift convergence reasonable
- Essential to use large N_{max}
  - Target wave function
  - Expansion of short-range parts of kernels
  - **IT NCSM** for the target makes it possible
- Need to include ^{16}O excited states (1p-1h…)
  - IT NCSM for excited states under way

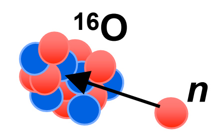




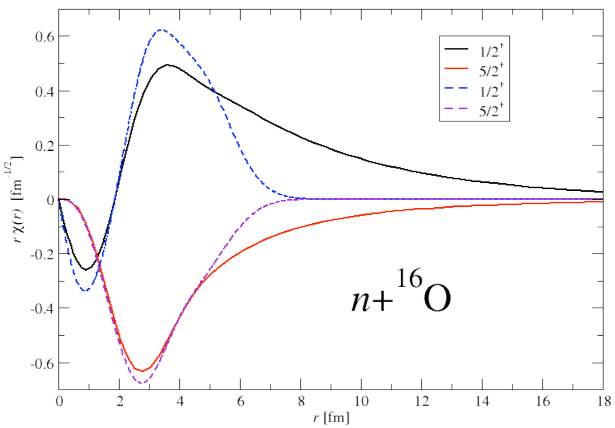
N_{max}=14

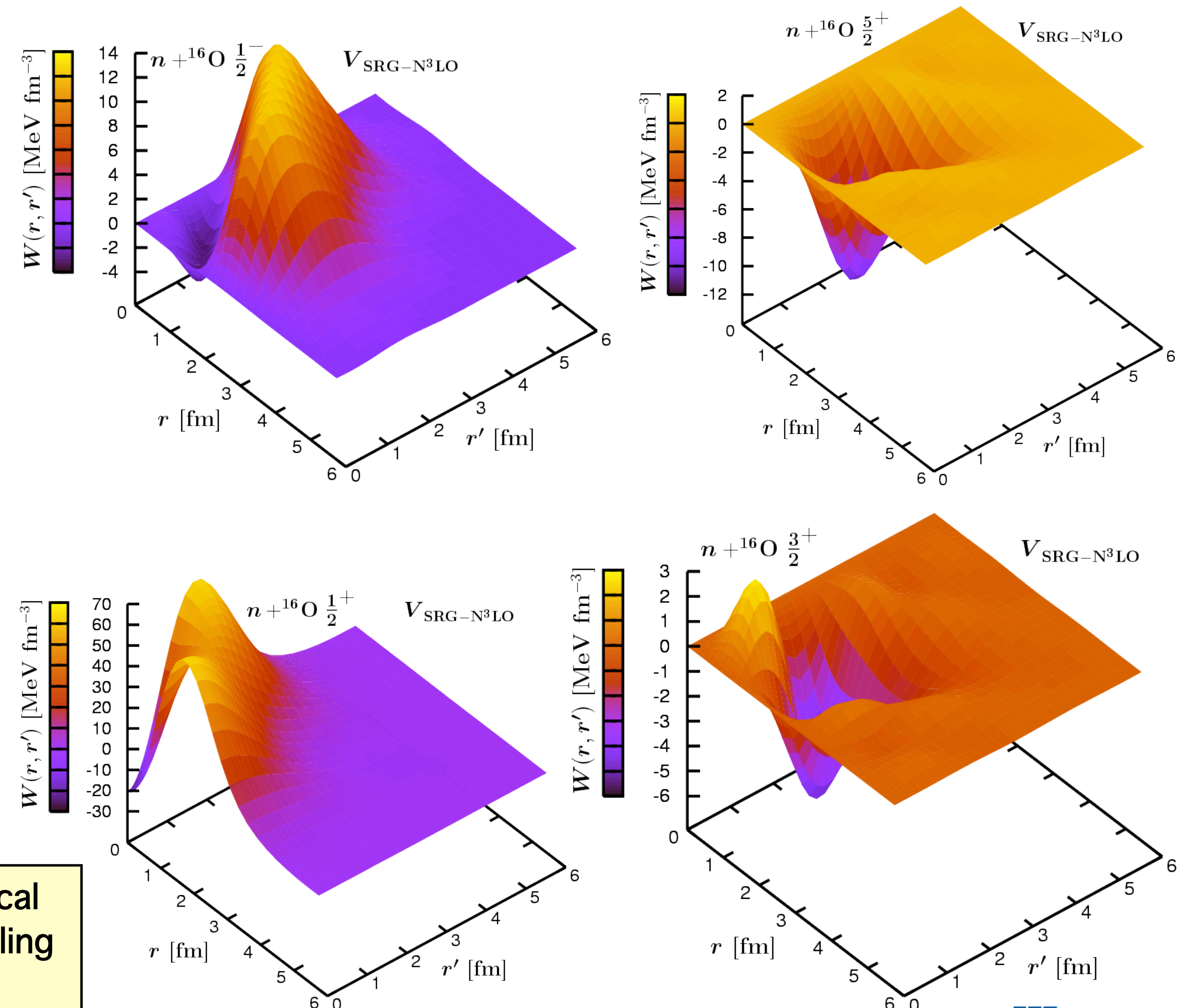
Combining the *ab initio* NCSM/RGM with the importance-truncated NCSM highly promising. Access to medium mass nuclei.

n-^{16}O scattering with SRG-N^{3}LO NN potential



- Orthogonalized NCSM/RGM equations:
  - Non-local nucleon-nucleus potential
    - Channel dependent
  - Wave functions





Direct connection to phenomenological reaction theory: Comparison of coupling potentials, wave functions

Computational issues

- The most computationally intensive:
  - NCSM/RGM with the target wave function expanded in Slater determinant basis (A>3)
    - Target wave functions calculations
      - Limit: Dimensions up to 10^8
      - Antoine
      - Codes developed from "Arizona" version of the MFD; MPI; up to 512 processors
    - One- and **two**-body transition densities from the target wave functions
      - TRDENS; MPI; up to 512 processors
      - Memory intensive: many combinations of operators in multi-shell HO basis (especially for eigenstates with J>0)
    - The kernel calculations from the densities is less challenging
  - NCSM/RGM with the target wave function expanded in Jacobi basis (A=3-5)
    - The kernel calculations
      - Sofia's code; MPI; up to 256 processors
- CS assistance sought for the TRDENS development and optimization

Past year publications citing UNEDF

PRL **99**, 092501 (2007) PHYSICAL REVIEW LETTERS week ending 31 AUGUST 2007

Ab Initio **Study of ^{40}Ca with an Importance-Truncated No-Core Shell Model**

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(Received 27 May 2007; published 29 August 2007)

We propose an importance truncation scheme for no-core shell model or configuration interaction approaches, which enables converged calculations for nuclei well beyond the *p* shell. It is based on an *a priori* measure for the importance of individual basis states constructed by means of many-body perturbation theory. Only the physically relevant states of the no-core model space are considered, which leads to a dramatic reduction of the basis dimension. We analyze the validity and efficiency of this truncation scheme using different realistic nucleon-nucleon interactions and compare to conventional no-core shell model calculations for ^{4}He and ^{16}O. Then, we present first converged calculations for the ground state of ^{40}Ca within no-core model spaces including up to $16\hbar\Omega$ excitations using realistic low-momentum interactions. The scheme is universal and can be easily applied to other quantum many-body problems.

Nuclear Electric Dipole Moment of ^{3}He

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arXiv:0804.3815; accepted in PLB

Few Body Syst (2007) 41: 117–140
DOI 10.1007/s00601-007-0193-3
Printed in The Netherlands

Few-Body Systems

Local three-nucleon interaction from chiral effective field theory

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Received 3 August 2007; Accepted 18 October 2007; Published online 30 November 2007

Abstract The three-nucleon (*NNN*) interaction derived within the chiral effective field theory at the next-to-next-to-leading order (N^{2}LO) is regulated with a function depending on the magnitude of the momentum transfer. The regulated *NNN* interaction is then local in the coordinate space, which is advantageous for some many-body techniques. Matrix elements of the local chiral *NNN* interaction are evaluated in a three-nucleon basis. Using the *ab initio* no-core shell model (NCSM) the *NNN* matrix elements are employed in ^{3}H and ^{4}He bound-state calculations.

Ab Initio Many-Body Calculations of n-^{3}H, n-^{4}He, p-^{3,4}He, and n-^{10}Be Scattering

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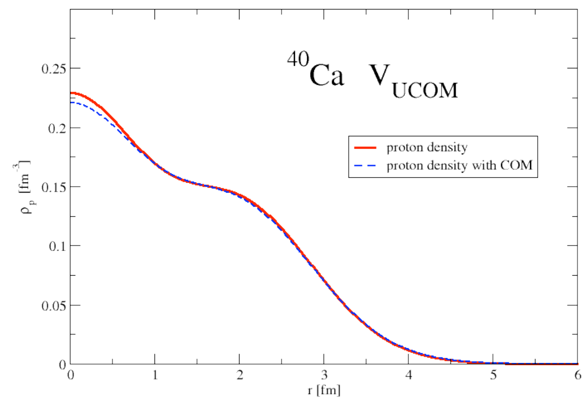
(Dated: April 9, 2008)

arXiv:0804.1560; submitted to PRL

Past year accomplishments and future plans

- Benchmark calculations for ^{7}Li, ^{9}Be and ^{12}C with mSSC V8’ NN potential
- Development of *ab initio* many-body reaction theory by merging the NCSM and the RGM
  - Results with NN potentials used by UNEDF collaboration
    - *n*-^{4}He (*p*-^{4}He) with SRG-N^{3}LO, SRG-AV18, mSSC V8’
    - *n*-^{12}C with mSSC V8’
    - *n*-^{16}O with SRG-N^{3}LO using the importance-truncated NCSM
    - Calculation of nucleon-nucleus non-local potentials
  - Bottleneck: Target wave-function and two-body density calc.
- ^{40}Ca with 4p-4h IT NCSM
- Development of the TRDENS transition density code
  - Used for the NCSM/RGM (one- and two-body) and other
  - MPI, memory intensive, CS assistance welcome
- LLNL Grand Challenge Award: 25 kCPU hours per week



- Year 2: Further work on non-local densities
- Year 3: Deuteron projectile within NCSM/RGM; nucleon scattering on medium-mass nuclei including excited states (IT NCSM); *A*=12 nuclei with chiral EFT NN+NNN
- Year 4,5: Realistic non-local potentials for nucleon-nucleus, deuteron-nucleus, connection to phenomenological reaction theory
- High-profile science: Capture reactions - ^{3}He(α,γ)^{7}Be, alpha-clustering