Nuclear structure and dynamics from chiral two- and three-nucleon forces

Tsukuba-CCS workshop on “microscopic theories of nuclear structure and dynamics”

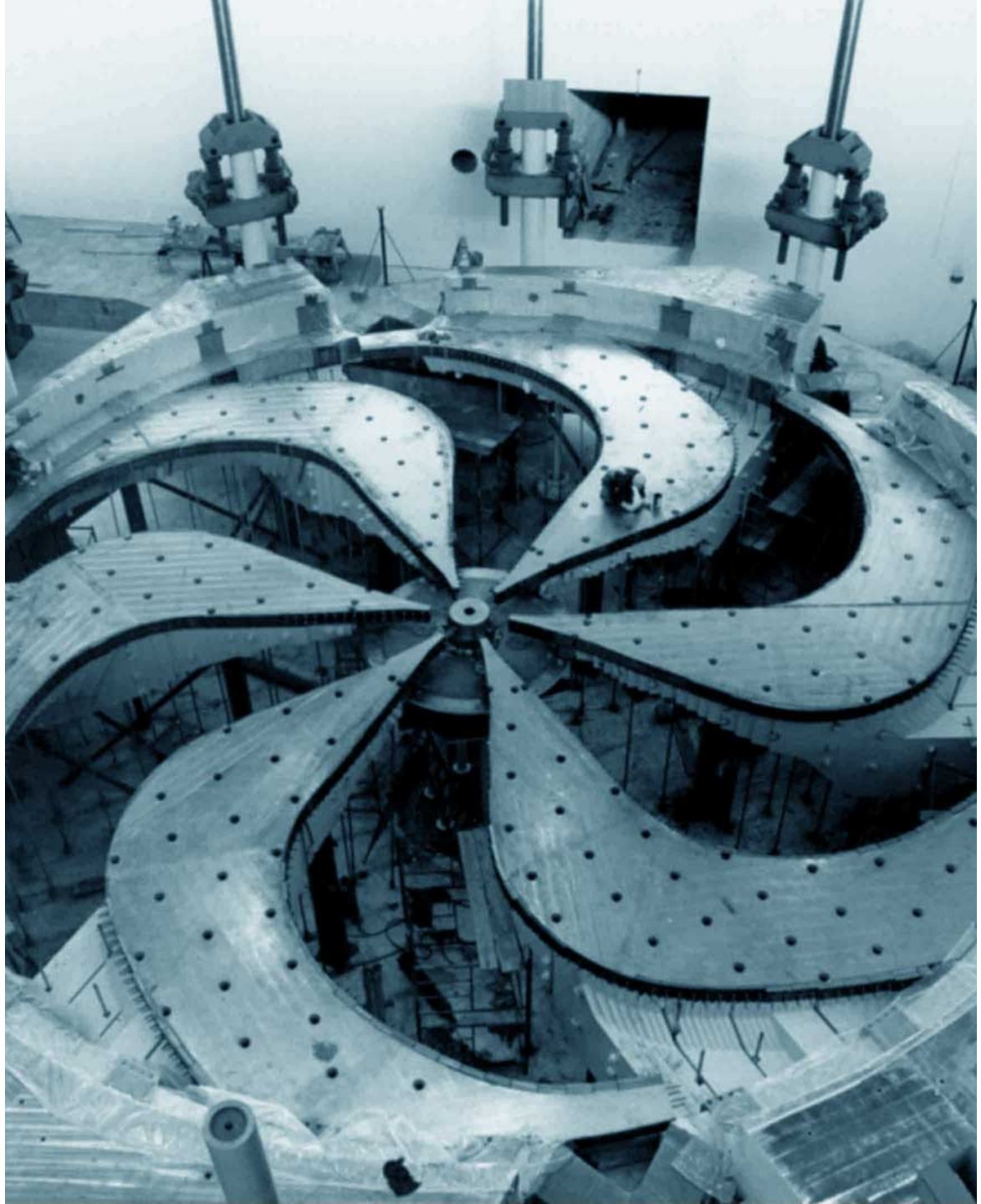
Center for Computational Sciences (CCS),
University of Tsukuba, Japan, December 10-12, 2018

Petr Navratil

TRIUMF

Collaborators: S. Quaglioni (LLNL), G. Hupin (Orsay), M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF), M. Gennari (U Waterloo), J. Dohet-Eraly (ULB)

2018-12-12

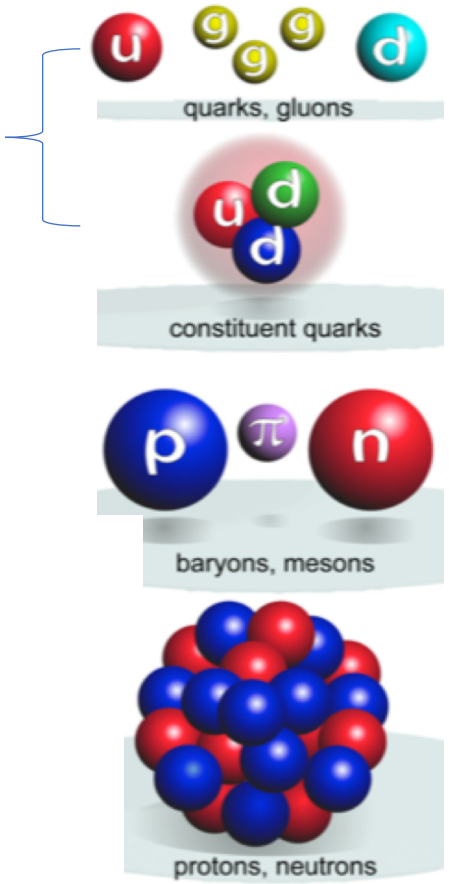


Outline

- Introduction to *ab initio* nuclear theory
- No-Core Shell Model with Continuum (NCSMC)
- ^{11}Be parity inversion in low-lying states, photo-dissociation
- Structure of the halo *sd*-shell nucleus ^{15}C

First principles or *ab initio* nuclear theory

Quantum Chromodynamics (QCD)



Genuine *Ab Initio*

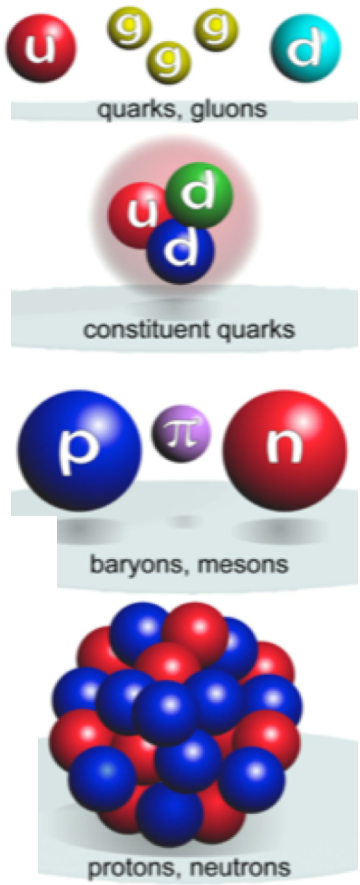
First principles or *ab initio* nuclear theory – what we do at present

Quantum Chromodynamics (QCD)

Chiral Effective Field Theory (parameters fitted to NN data)

Current *ab anitio* nuclear theory

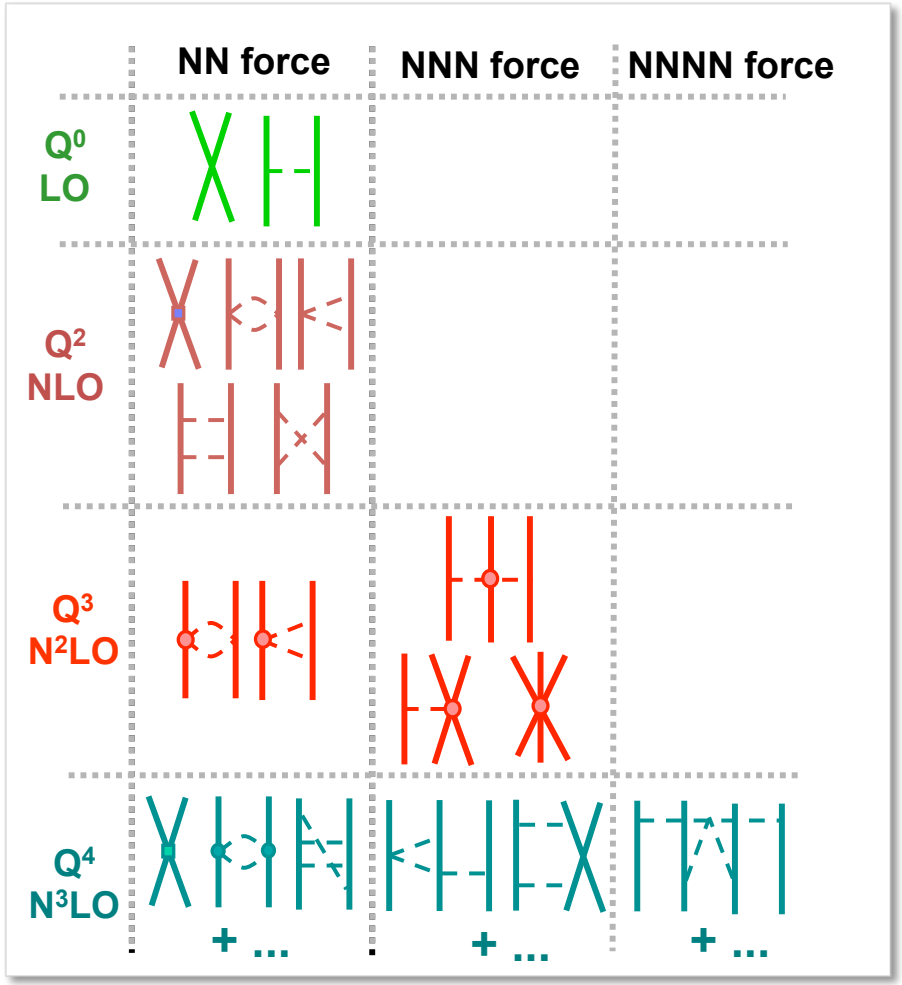
$$H\,\Psi^{(A)} = E\,\Psi^{(A)}$$



- *Ab initio*
  - ✧ Degrees of freedom: Nucleons
  - ✧ All nucleons are active
  - ✧ Exact Pauli principle
  - ✧ Realistic inter-nucleon interactions
    - ✧ Accurate description of NN (and 3N) data
  - ✧ Controllable approximations

Chiral Effective Field Theory

- Inter-nucleon forces from chiral effective field theory
  - Based on the symmetries of QCD
    - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
    - Degrees of freedom: nucleons + pions
  - Systematic low-momentum expansion to a given order (Q/Λ_χ)
  - Hierarchy
  - Consistency
  - Low energy constants (LEC)
    - Fitted to data
    - Can be calculated by lattice QCD



Λ_χ~1 GeV :
Chiral symmetry breaking scale

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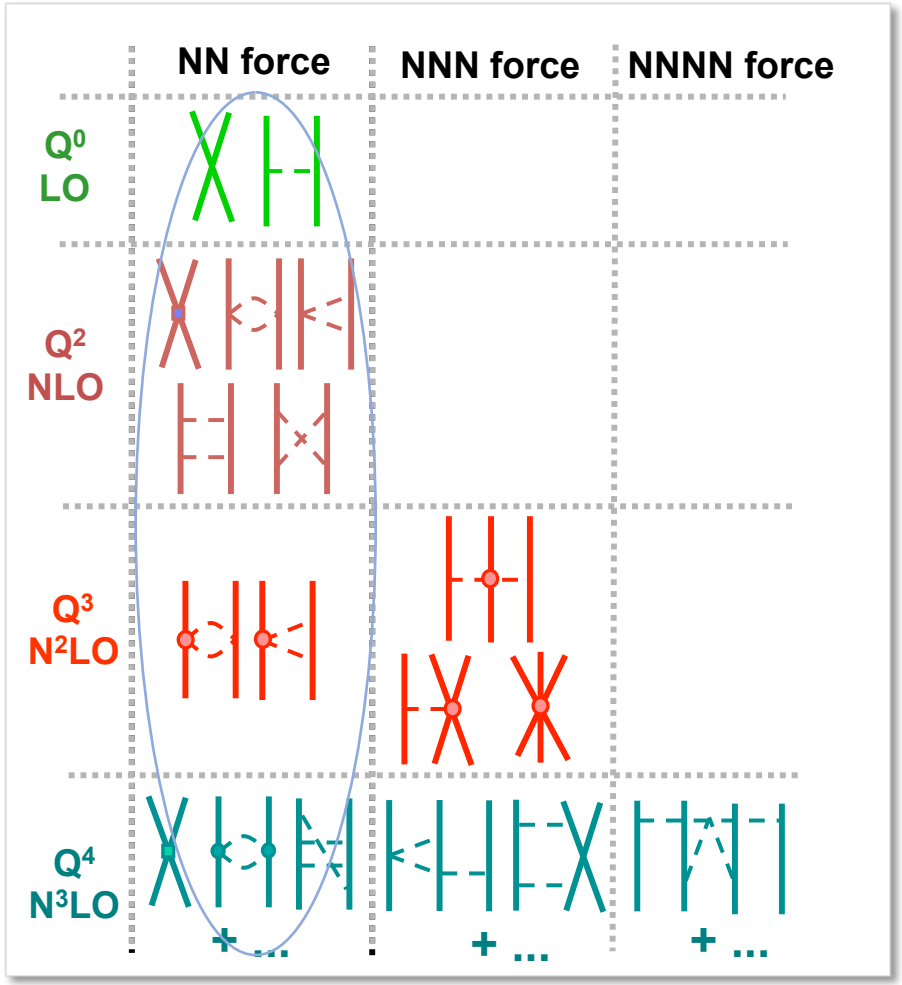

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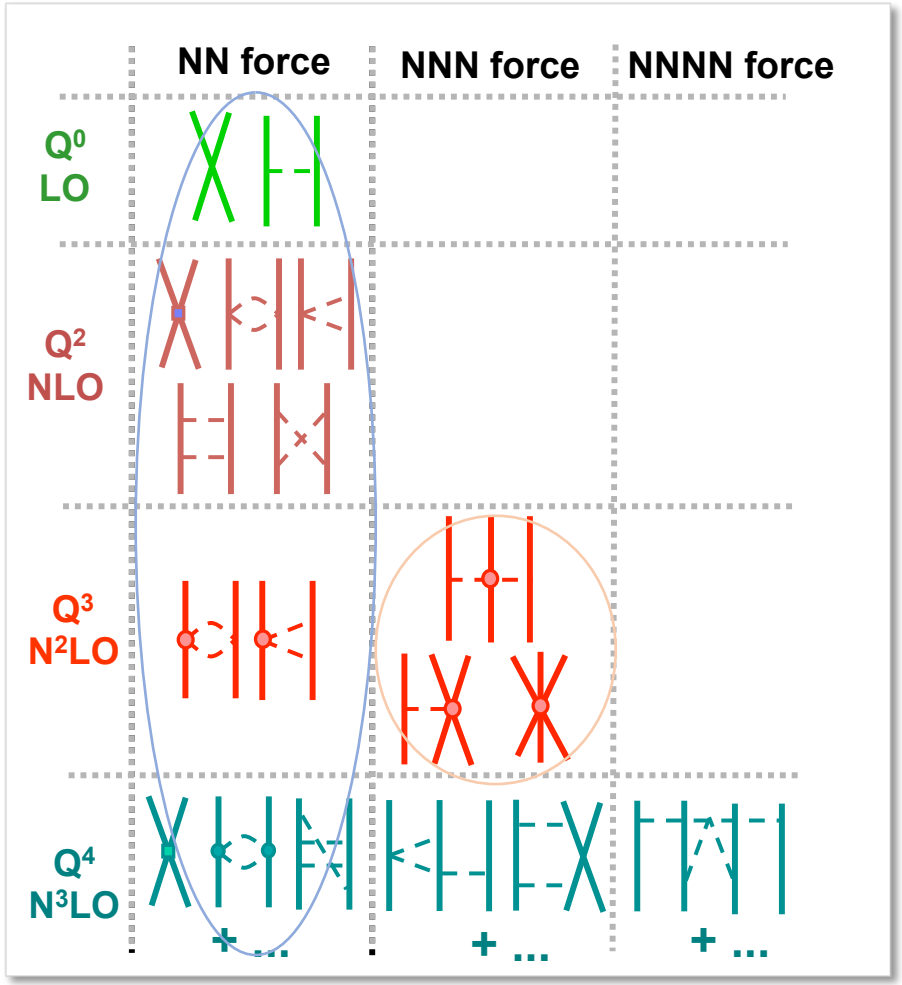

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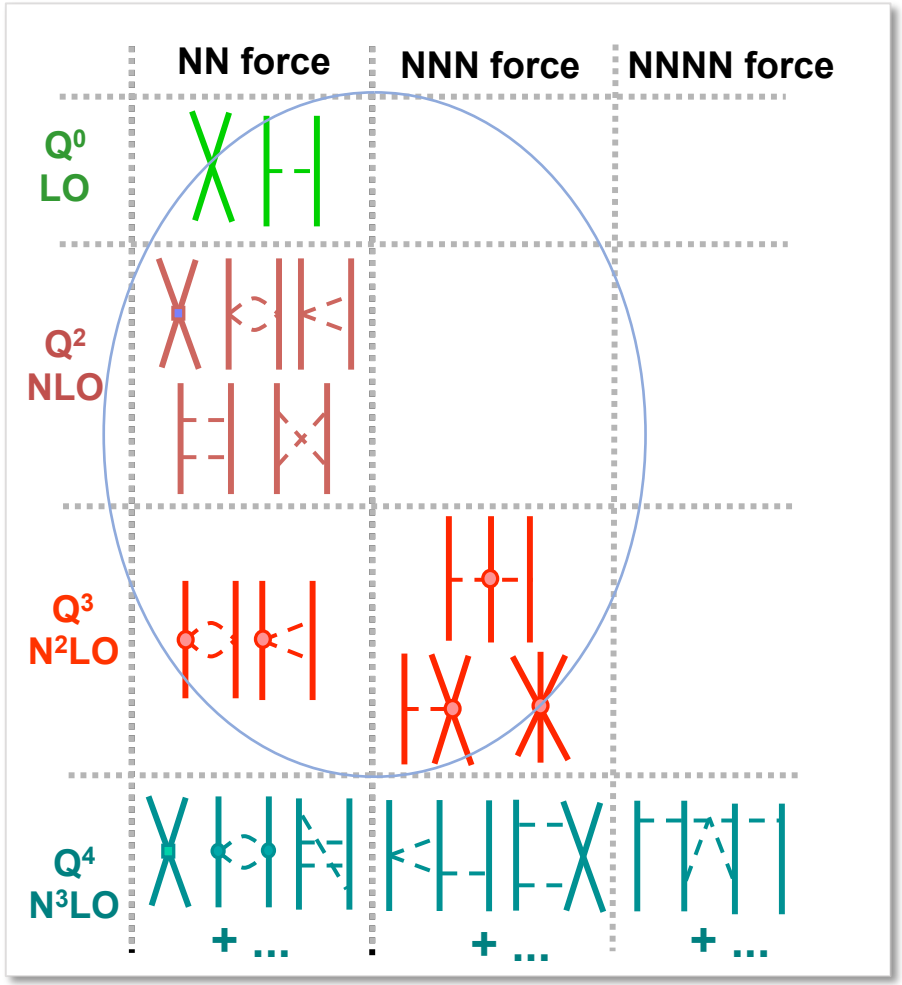
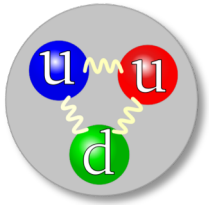
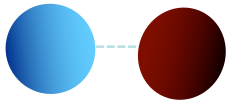
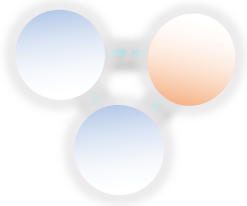


Λ_χ~1 GeV :
Chiral symmetry breaking scale

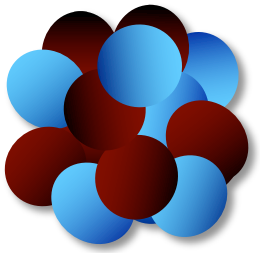
From QCD to nuclei







$$H|\Psi\rangle = E|\Psi\rangle$$



Low-energy QCD

NN+3N interactions from chiral EFT

…or accurate meson-exchange potentials

Unitary/similarity transformations

Identity or SRG or OLS or UCOM … Softens NN, induces 3N

Many-Body methods

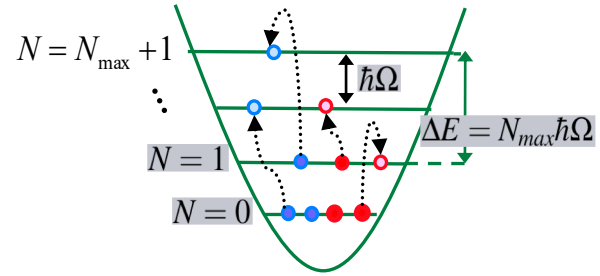
NCSM, NCSMC, CCM, SCGF, IM-SRG, GFMC, HH, Nuclear Lattice EFT…

Nuclear structure and reactions

Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

NCSM

- Basis expansion method
  - Harmonic oscillator (HO) basis truncated in a particular way ($N_{\max}$)
  - Why HO basis?
    - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ^{4}He, ^{16}O, ^{40}Ca)
    - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



$$(A)\ \Psi^{A} = \sum_{N=0}^{N_{\max}} \sum_{i} c_{Ni}\, \Phi^{HO}_{Ni}(\vec{\eta}_1, \vec{\eta}_2, \ldots, \vec{\eta}_{A-1})$$

$$(A)\ \Psi^{A}_{\mathrm{SD}} = \sum_{N=0}^{N_{\max}} \sum_{j} c^{\mathrm{SD}}_{Nj}\, \Phi^{HO}_{\mathrm{SD}\,Nj}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^{A}\, \varphi_{000}(\vec{R}_{CM})$$

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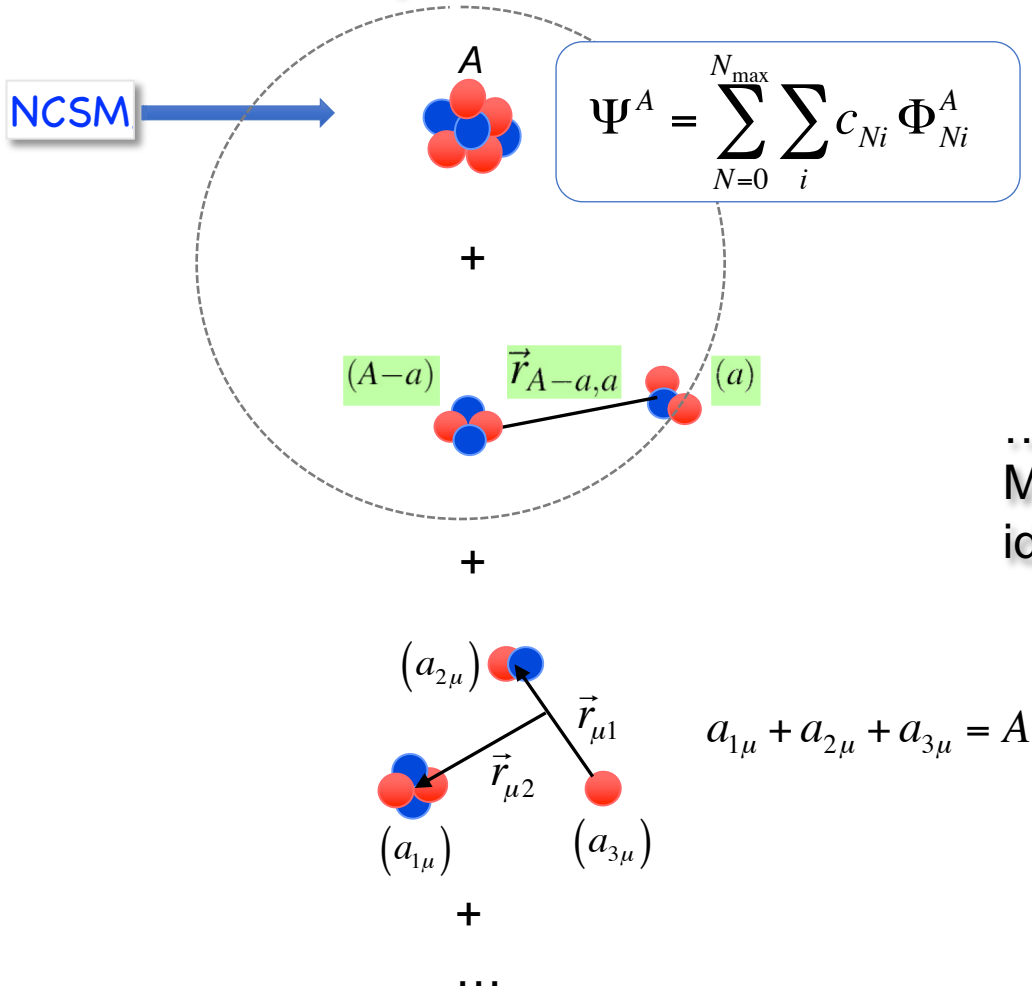
Review

Ab initio no core shell model

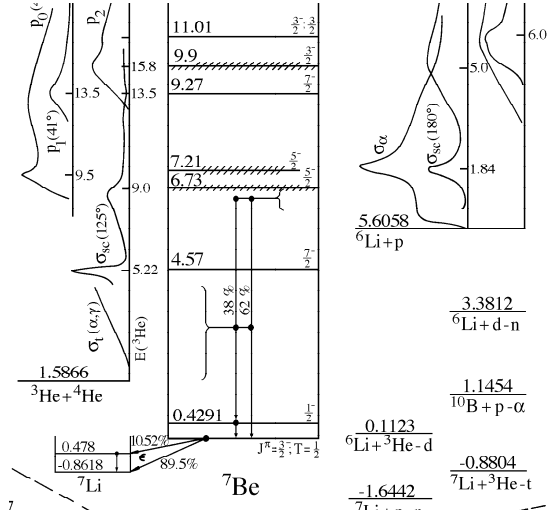
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

Extending no-core shell model beyond bound states

Include more many nucleon correlations…



…using the Resonating Group Method (RGM) ideas

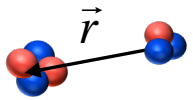


Unified approach to bound & continuum states; to nuclear structure & reactions

- No-core shell model (NCSM)
  - *A*-nucleon wave function expansion in the harmonic-oscillator (HO) basis
  - short- and medium range correlations
  - Bound-states, narrow resonances

NCSM

- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion, clusters described by NCSM
  - proper asymptotic behavior
  - long-range correlations



NCSM/RGM

- Most efficient: *ab initio* no-core shell model with continuum (NCSMC)

NCSMC

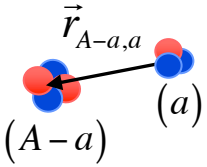
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A) \; , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}\,) \; \hat{A}_{\nu} \left| \; \vec{r} \; (a) \; , \nu \right\rangle$$

$(A-a)$

Unknowns

S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Binary cluster basis



- Working in partial waves ($\nu \equiv \{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\}$)

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \hat{A}_\nu \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle}_{\text{Target}} \underbrace{\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle}_{\text{Projectile}} \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{g_\nu^{J^\pi T}(r_{A-a,a})}{r_{A-a,a}}$$

- Introduce a dummy variable $\vec{r}$ with the help of the delta function

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle \right)^{(sT)} Y_\ell(\hat{r}) \right]^{(J^\pi T)} \delta(\vec{r} - \vec{r}_{A-a,a})\ r^2 dr\, d\hat{r}$$

  - Allows to bring the wave function of the relative motion in front of the antisymmetrizer

$$\sum_\nu \int d\vec{r}\ \gamma_\nu(\vec{r})\ \hat{A}_\nu \left| \vec{r}, (a), (A-a), \nu \right\rangle$$

Coupled NCSMC equations

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

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A) \right., \lambda \rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \left| \vec{r}\,, (a)\ (A-a) \right., \nu \rangle$$

$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

$E_{\lambda}^{NCSM}\ \delta_{\lambda\lambda'}$ — $\langle (A) | H\,\hat{A}_{\nu} | (a)\ (A-a) \rangle$ — $\delta_{\lambda\lambda'}$ — $\langle (A) | \hat{A}_{\nu} | (a)\ (A-a) \rangle$

$\langle (A-a)\ (a) | \hat{A}_{\nu'}\, H\, \hat{A}_{\nu} | (a)\ (A-a) \rangle$ — $\langle (A-a)\ (a) | \hat{A}_{\nu'}\, \hat{A}_{\nu} | (a)\ (A-a) \rangle$

Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for coupled channels

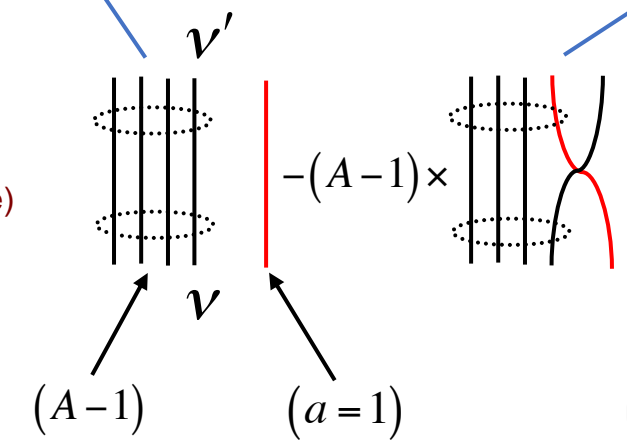
Norm kernel (Pauli principle): Single-nucleon projectile

$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \middle| \hat{A}_{\nu'} \hat{A}_{\nu} \middle| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \; (A-1) \;\; r' \;\; (a'=1) \right| \left(1 - \sum_{i=1}^{A-1} \hat{P}_{iA}\right) \left| \; (A-1) \;\; r \;\; (a=1) \right\rangle$$

$$N^{J^\pi T}_{\nu'\nu}(r',r) = \delta_{\nu'\nu} \frac{\delta(r'-r)}{r'r} - (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \left\langle \Phi^{J^\pi T}_{\nu' n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{J^\pi T}_{\nu n} \right\rangle$$

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

Direct term:
Treated exactly!
(in the full space)



$-(A-1)\times$

Exchange term:
Obtained in the model space!
(Many-body correction due to
the exchange part of the inter-
cluster antisymmetrizer)

Trick #1

$$\frac{\delta(r - r_{A-a,a})}{r\, r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

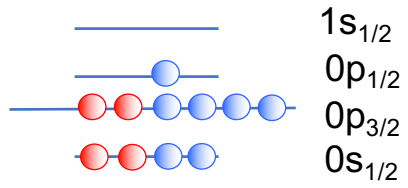
Trick #2

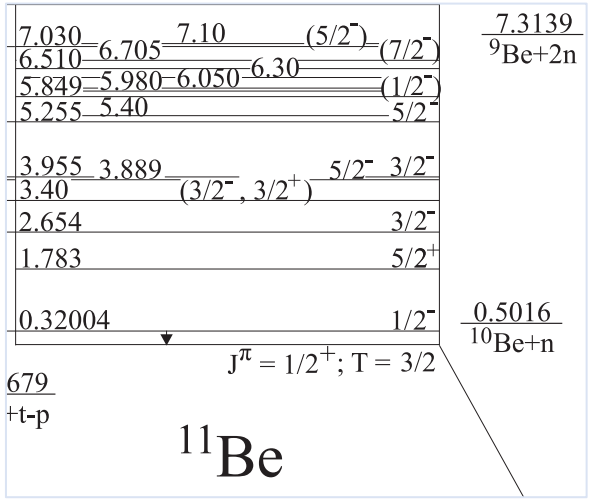
Target wave functions expanded in the SD basis, the CM motion exactly removed

Neutron-rich halo nucleus ^{11}Be

- Z=4, N=7
  - In the shell model picture g.s. expected to be $J^{\pi}=1/2^-$
    - Z=6, N=7 ^{13}C and Z=8, N=7 ^{15}O have $J^{\pi}=1/2^-$ g.s.
  - In reality, ^{11}Be g.s. is **$J^{\pi}=1/2^+$** - parity inversion
  - Very weakly bound: E_{th}=-0.5 MeV
    - Halo state – dominated by ^{10}Be-n in the *S*-wave
  - The $1/2^-$ state also bound – only by 180 keV

- Can we describe ^{11}Be in *ab initio* calculations?
  - Continuum must be included
  - Does the 3N interaction play a role in the parity inversion?

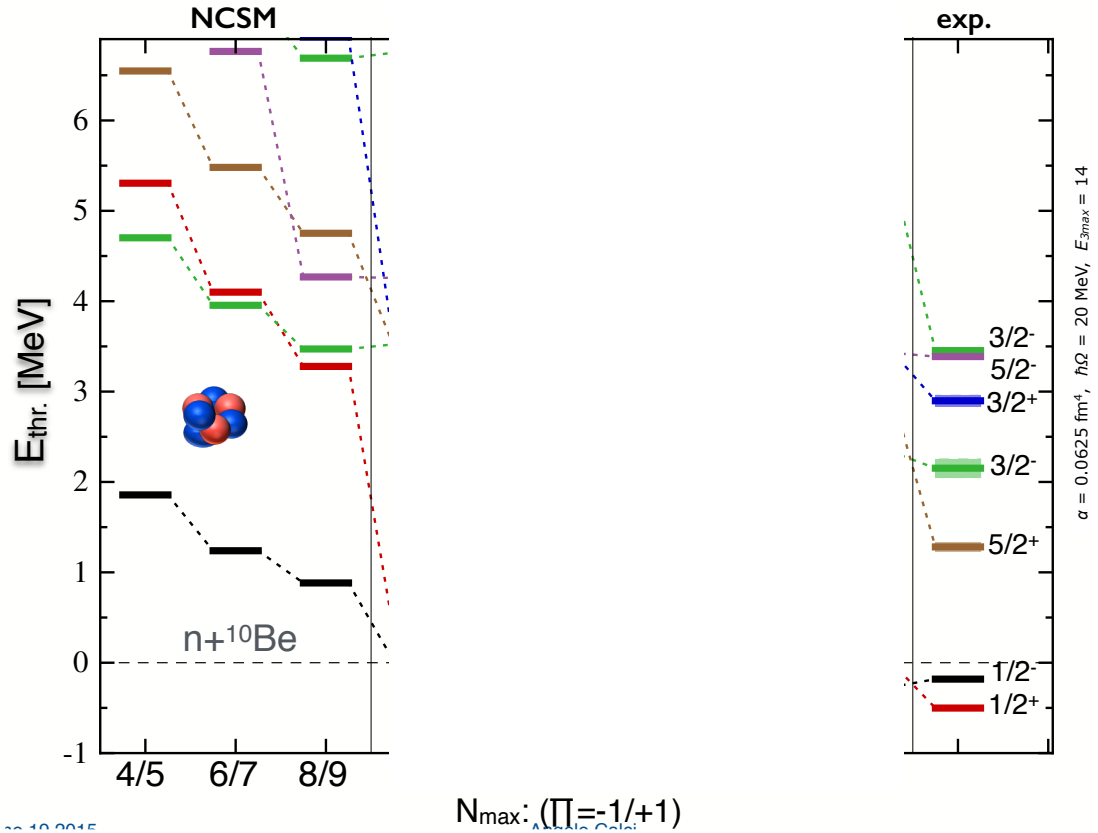




Structure of ^{11}Be from chiral NN+3N forces

17

- NCSMC calculations **including chiral 3N** (N^3LO NN+N^2LO 3NF400, NNLOsat)
  - n-^{10}Be + ^{11}Be
    - ^{10}Be: 0^+, 2^+, 2^+ NCSM eigenstates
    - ^{11}Be: ≥6 π = -1 and ≥3 π = +1 NCSM eigenstates



A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, PRL 117, 242501 (2016)

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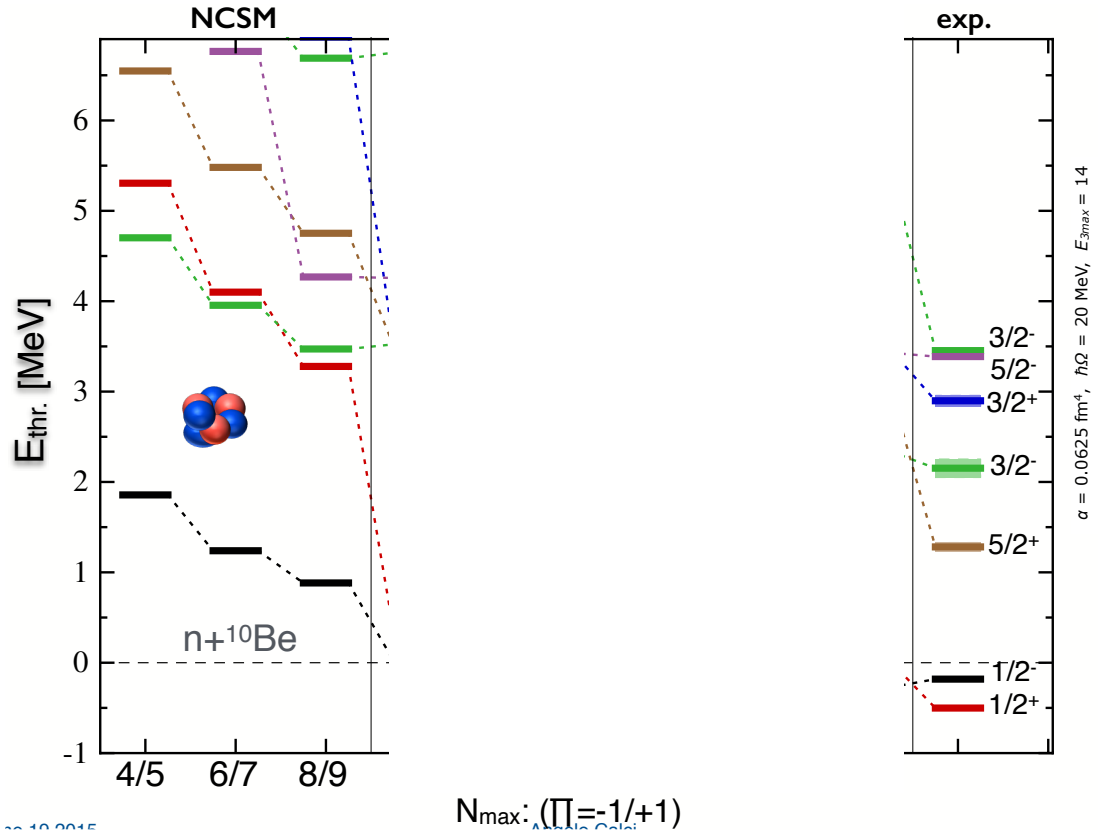
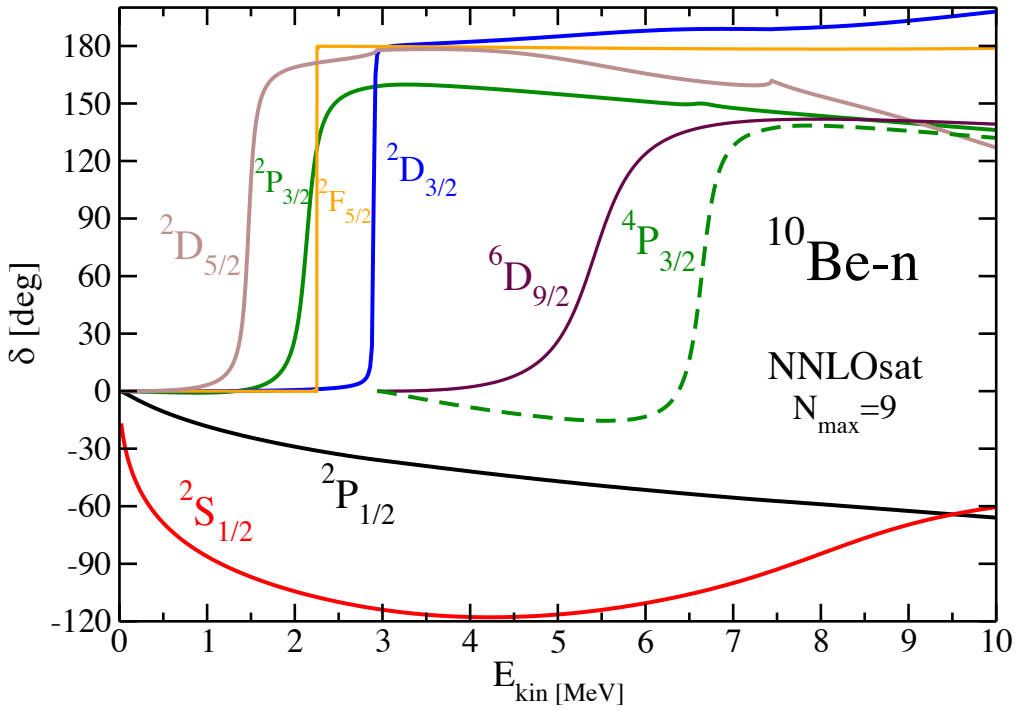


N_{max}: (∏=-1/+1)



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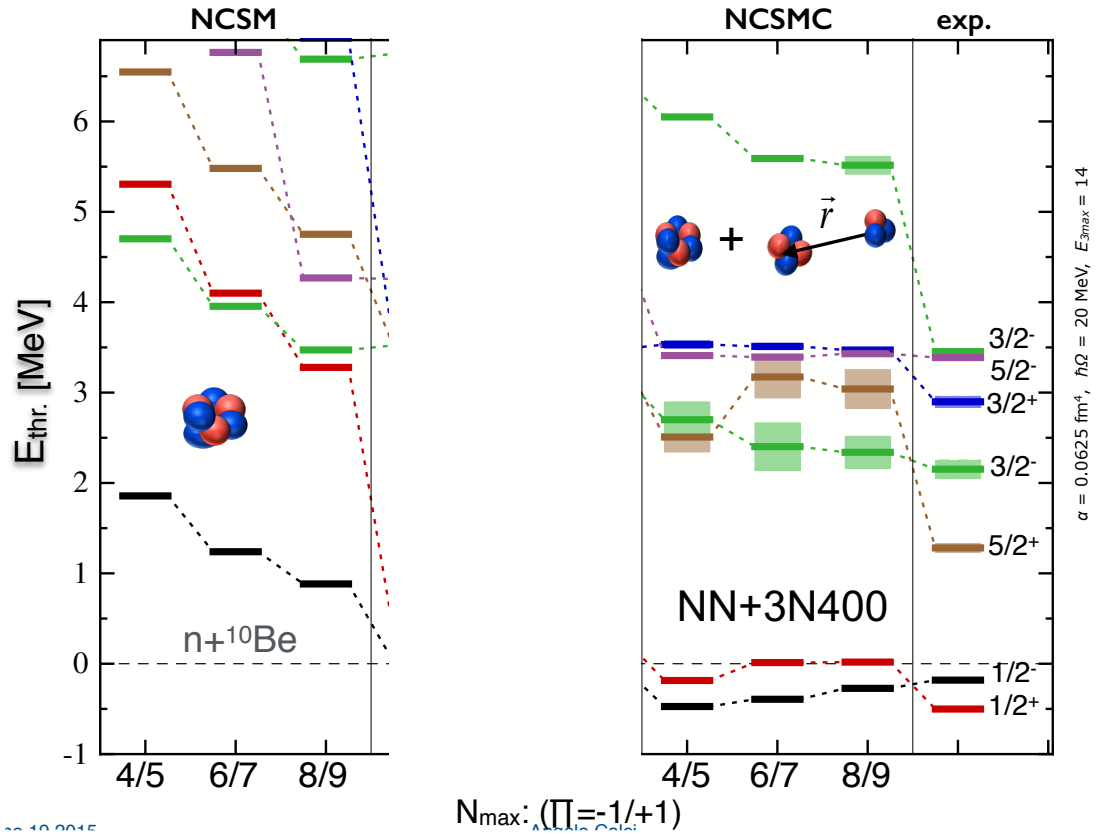

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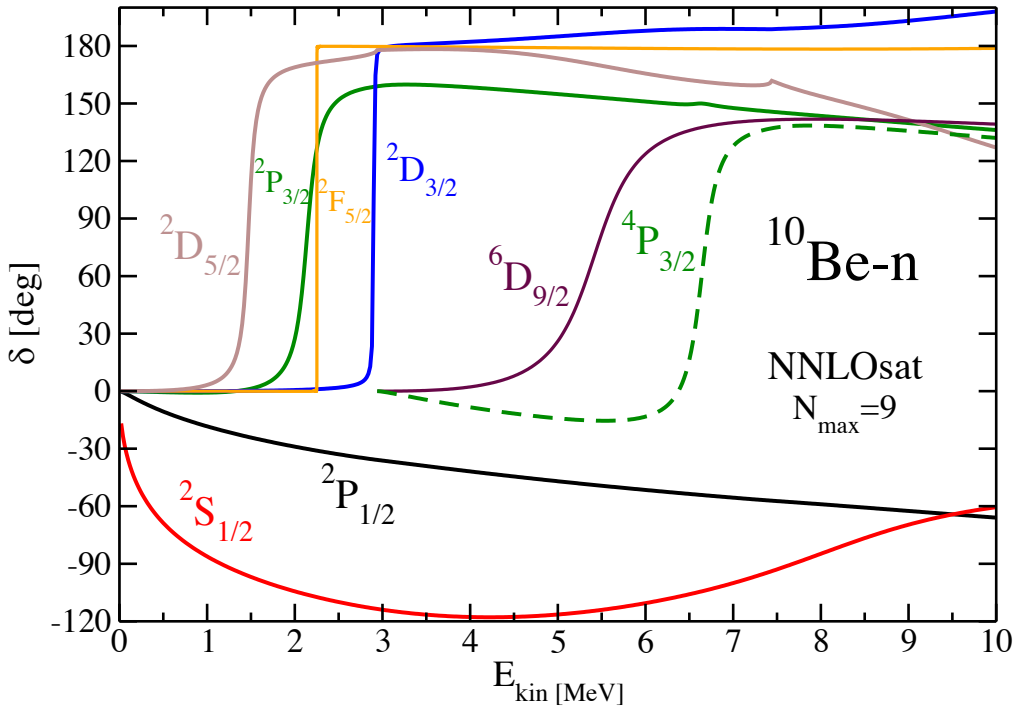

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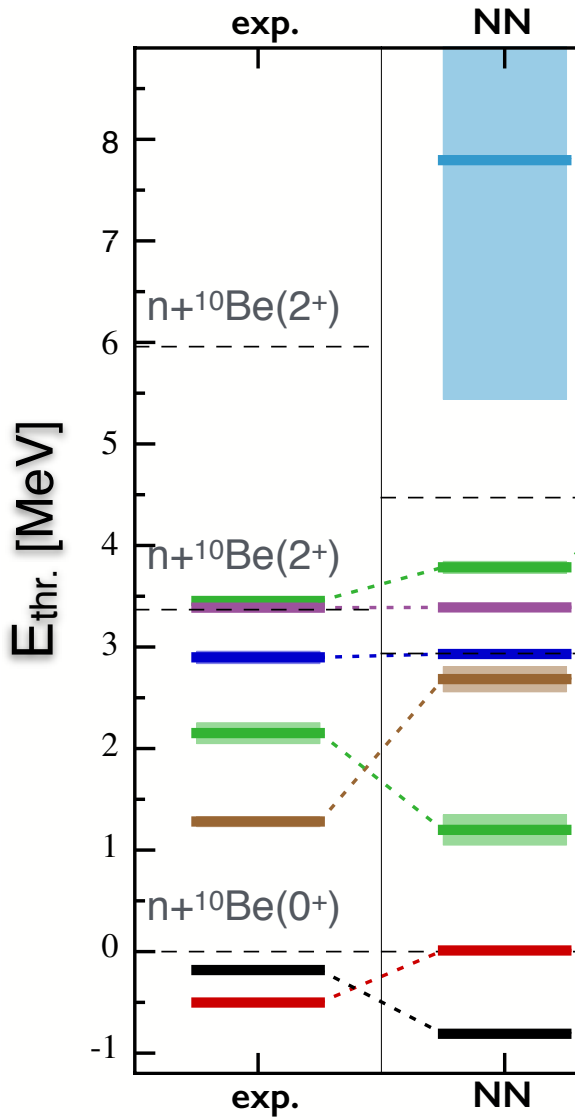
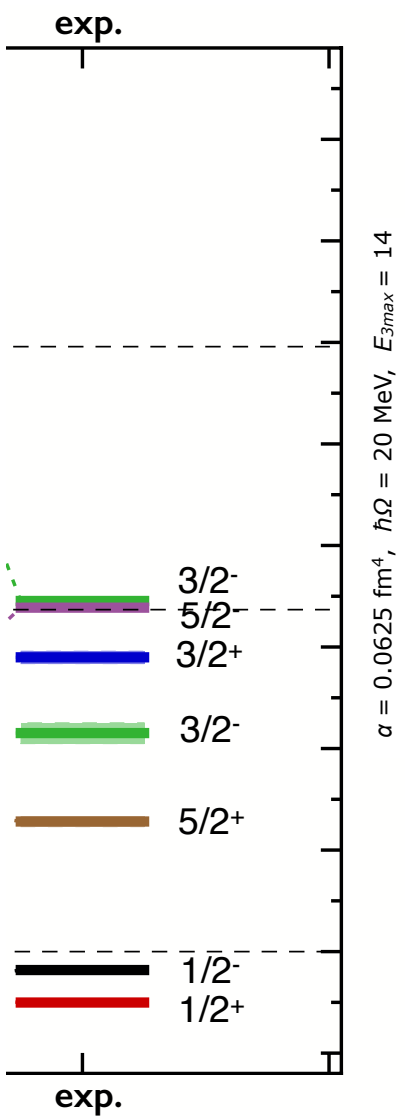
^{11}Be within NCSMC: Discrimination among chiral nuclear forces





α = 0.0625 fm^4, $\hbar\Omega$ = 20 MeV, E_{3max} = 14

A. Calci, P. Navratil, R. Roth, J. Dohet-Eraly, S. Quaglioni, G. Hupin, PRL 117, 242501 (2016)

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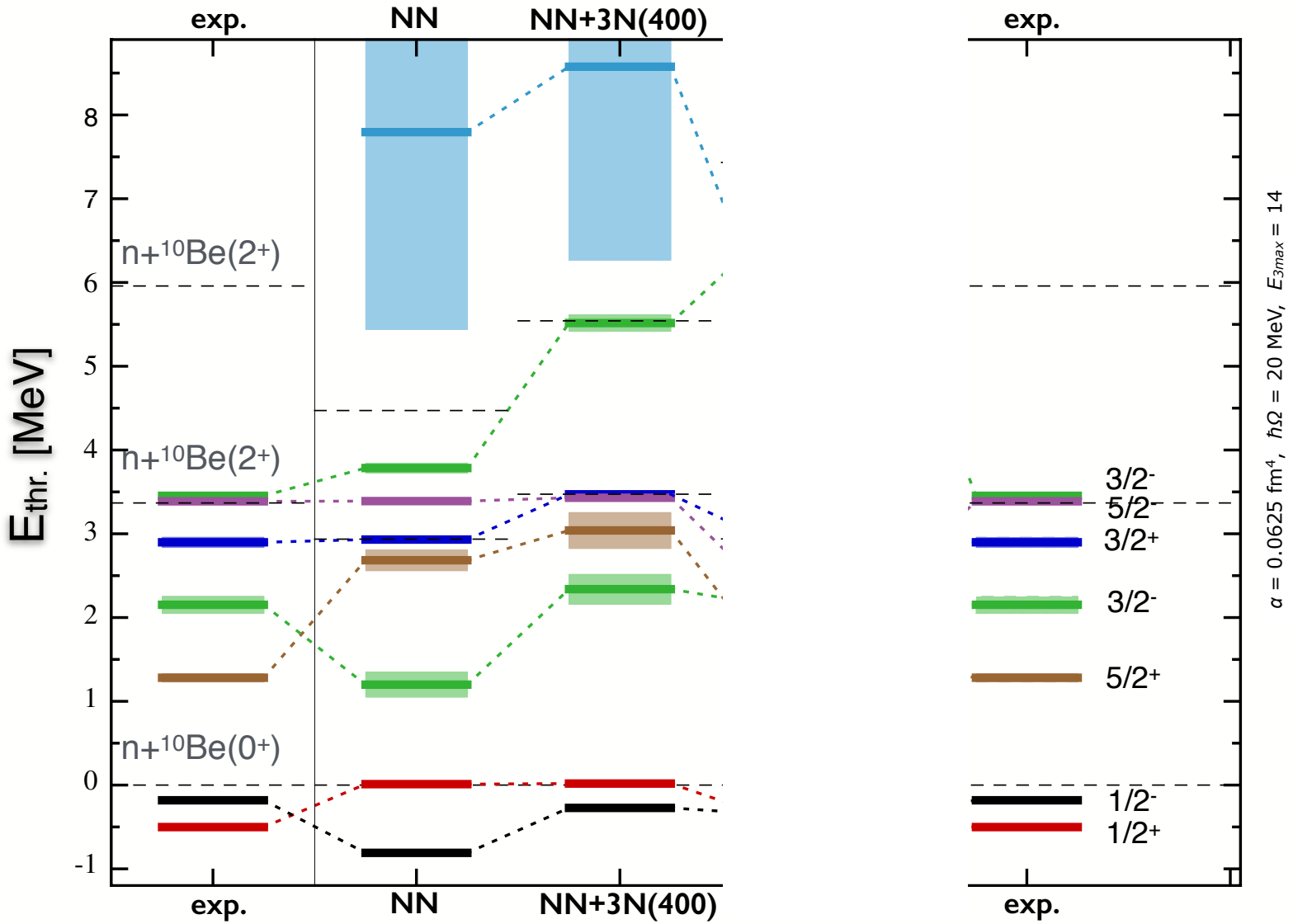

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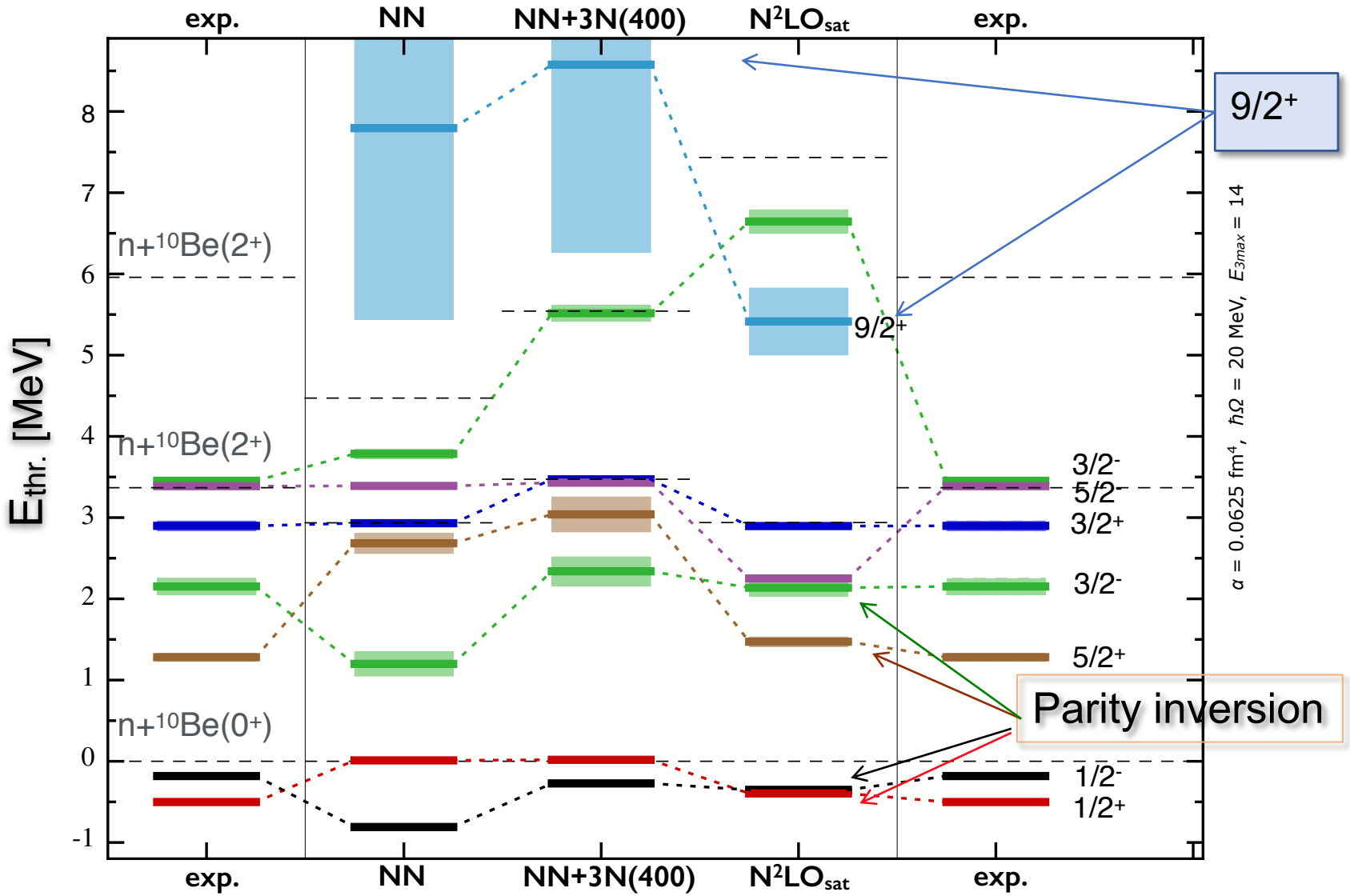

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E1 transitions in NCSMC

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| (A), \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\, \gamma_{\nu}(\vec{r})\, \hat{A}_{\nu} \left| (A-a) \; \vec{r} \; (a), \nu \right\rangle$$

$$\vec{E}1 = e \sum_{i=1}^{A-a} \frac{1+\tau_i^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(A-a)}_{\text{c.m.}} \right) + e \sum_{j=A-a+1}^{A} \frac{1+\tau_j^{(3)}}{2} \left(\vec{r}_i - \vec{R}^{(a)}_{\text{c.m.}} \right) + e \frac{Z_{(A-a)} a - Z_{(a)}(A-a)}{A} \vec{r}_{A-a,a} \,.$$

$$\begin{aligned} M^{E1}_{fi} = & \sum_{\lambda\lambda'} c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \vec{E}1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_{\lambda} \\ & + \sum_{\lambda'\nu} \int drr^2 \, c^{*f}_{\lambda'} \langle A\lambda' J_f^{\pi_f} T_f || \vec{E}1 \hat{\mathcal{A}}_{\nu} || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_{\nu}(r)}{r} \\ & + \sum_{\lambda\nu'} \int dr' r'^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \vec{E}1 || A\lambda J_i^{\pi_i} T_i \rangle \, c^i_{\lambda} \\ & + \sum_{\nu\nu'} \int dr' r'^2 \int drr^2 \frac{\gamma^{*f}_{\nu'}(r')}{r'} \langle \Phi^f_{\nu' r'} || \hat{\mathcal{A}}_{\nu'} \vec{E}1 \hat{\mathcal{A}}_{\nu} || \Phi^i_{\nu r} \rangle \, \frac{\gamma^i_{\nu}(r)}{r} \end{aligned}$$

Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)

PRL 117, 242501 (2016) PHYSICAL REVIEW LETTERS week ending 9 DECEMBER 2016

Can *Ab Initio* Theory Explain the Phenomenon of Parity Inversion in ^{11}Be?

Angelo Calci,[1,*] Petr Navrátil,[1,†] Robert Roth,[2] Jérémy Dohet-Eraly,[1,‡] Sofia Quaglioni,[3] and Guillaume Hupin[4,5]

NCSMC phenomenology

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

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r}\,)\ \hat{A}_{\nu} \left| {}^{(A-a)}\ \vec{r}\ {}^{(a)}, \nu \right\rangle$$

E_λ^{NCSM} energies treated as adjustable parameters

Cluster excitation energies set to experimental values

$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

$E_\lambda^{NCSM}\ \delta_{\lambda\lambda'}$ — $\left\langle {}^{(A)} \left| H\,\hat{A}_{\nu} \right| {}^{(a)}\ r\ {}^{(A-a)} \right\rangle$

$\delta_{\lambda\lambda'}$ — $\left\langle {}^{(A)} \left| \hat{A}_{\nu} \right| {}^{(a)}\ r\ {}^{(A-a)} \right\rangle$

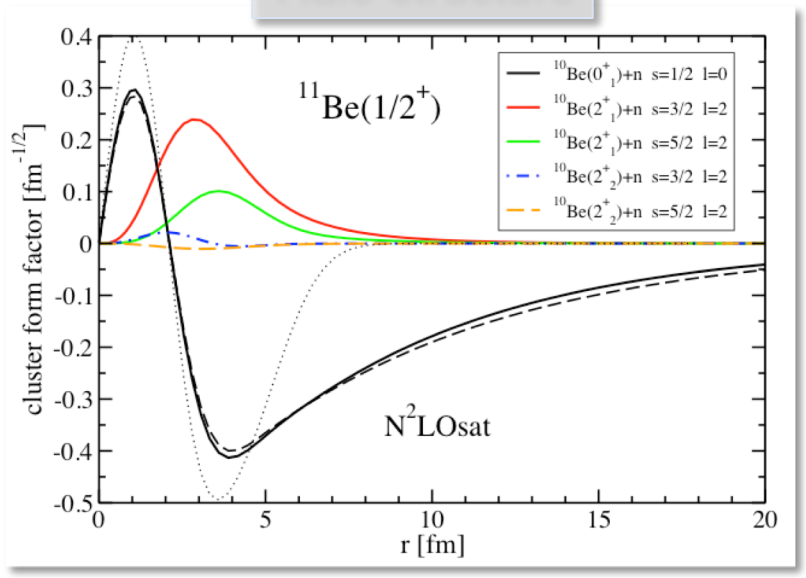
$\left\langle {}^{(A-a)}\ r'\ {}^{(a)} \left| \hat{A}_{\nu'}\, H\, \hat{A}_{\nu} \right| {}^{(a)}\ r\ {}^{(A-a)} \right\rangle$

$\left\langle {}^{(A-a)}\ r'\ {}^{(a)} \left| \hat{A}_{\nu'}\, \hat{A}_{\nu} \right| {}^{(a)}\ r\ {}^{(A-a)} \right\rangle$

Photo-disassociation of ^{11}Be

Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^+ \rightarrow 1/2^-$) [e^2 fm^2]	0.0005	0.117	0.102(2)

Halo structure



cluster form factor

$$= r \left\langle \Phi^{J^\pi T}_{vr} \middle| \hat{A}_\nu \middle| \psi^{J^\pi T} \right\rangle$$

$$\left| \Phi^{J^\pi T}_{vr} \right\rangle = \left[\left(\left| {}^{10}\mathrm{Be}\ \alpha_1 I_1^{\pi_1} T_1 \right\rangle \left| n\, \tfrac{1}{2}^+\, \tfrac{1}{2} \right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{10,1}) \right]^{(J^\pi T)} \frac{\delta(r - r_{10,1})}{r r_{10,1}}$$

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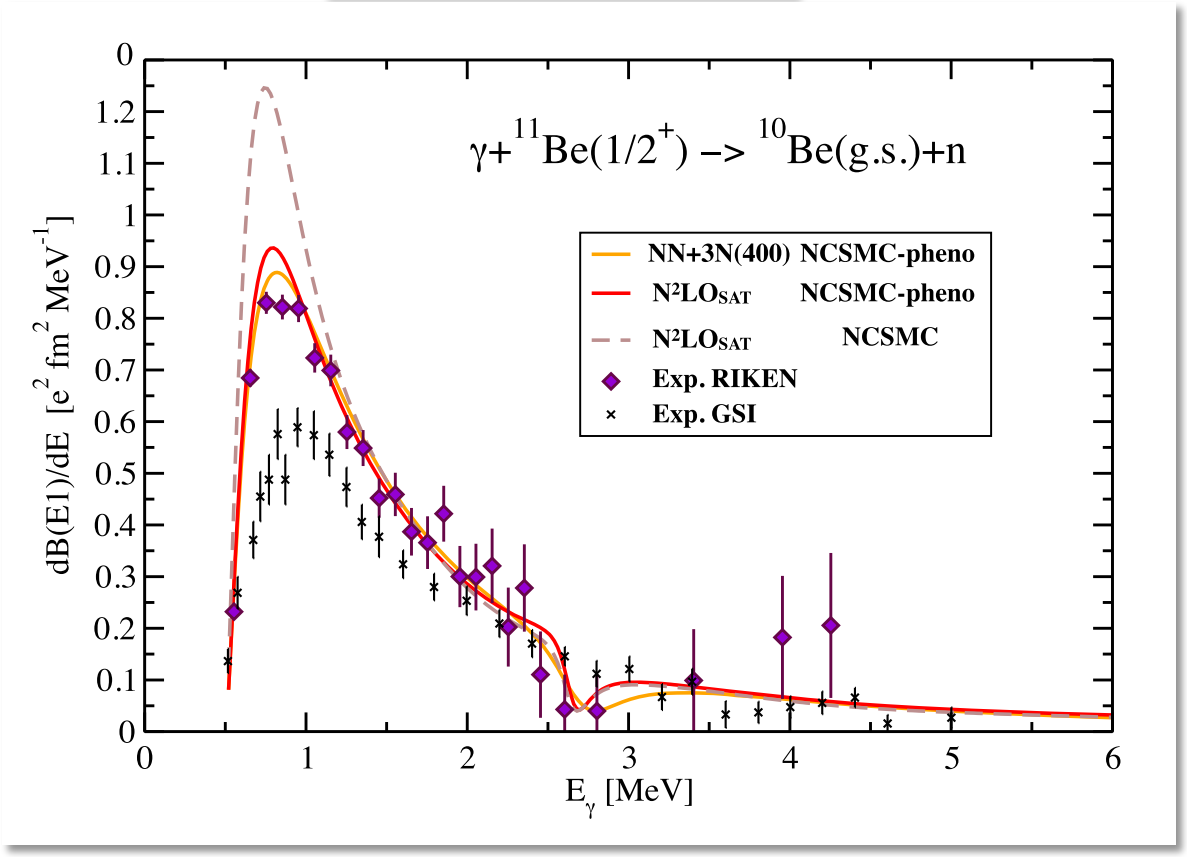
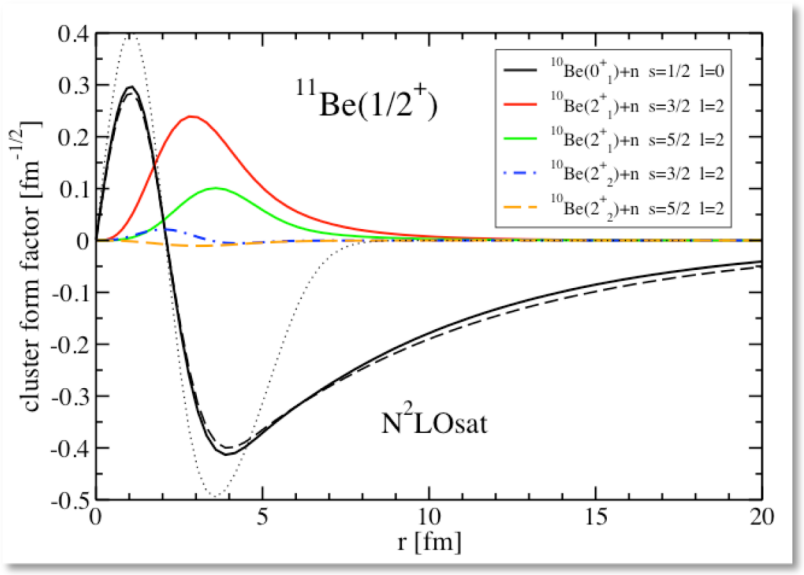
Bound to continuum



NCSMC wave functions of ^{11}Be used as input for other studies



PHYSICAL REVIEW C **98**, 054602 (2018)

Systematic analysis of the peripherality of the ^{10}Be(d, p)^{11}Be transfer reaction and extraction of the asymptotic normalization coefficient of ^{11}Be bound states

J. Yang[1,2,*] and P. Capel[1,3,†]

PHYSICAL REVIEW C **98**, 034610 (2018)

Dissecting reaction calculations using halo effective field theory and *ab initio* input

P. Capel,[1,2,3,4,*] D. R. Phillips,[5,3,4,†] and H.-W. Hammer[3,4,‡]

Reliable extraction of the $dB(\mathrm{E1})/dE$ for ^{11}Be from its breakup at 520 MeV/nucleon

Laura Moschini[1,*] and Pierre Capel[2,1,†]

arXiv:1807.07537

PRL **117,** 242501 (2016) PHYSICAL REVIEW LETTERS week ending 9 DECEMBER 2016

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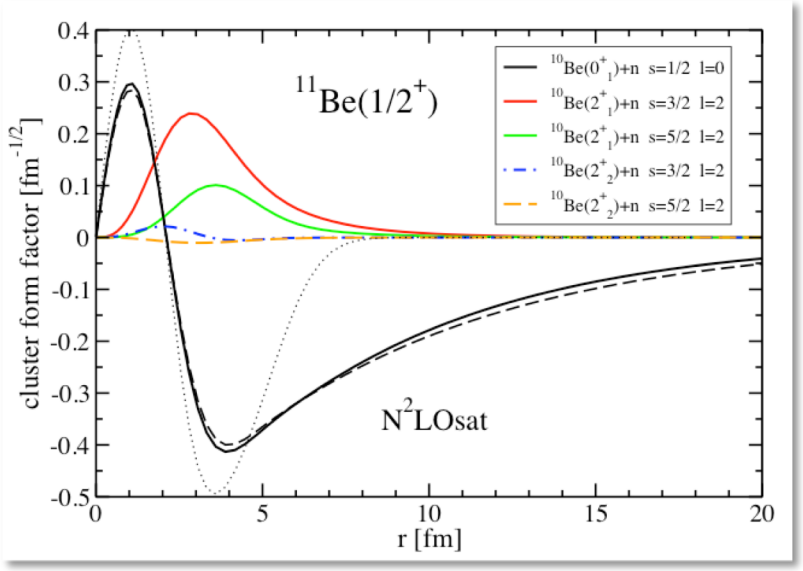
NCSMC wave functions of ^{11}Be used as input for other studies



Neutron disappearance inside the nucleus

H. Ejiri[1], J.D. Vergados[2]

arXiv:1805.04477; accepted in JPG

PRL **117,** 242501 (2016) PHYSICAL REVIEW LETTERS week ending 9 DECEMBER 2016

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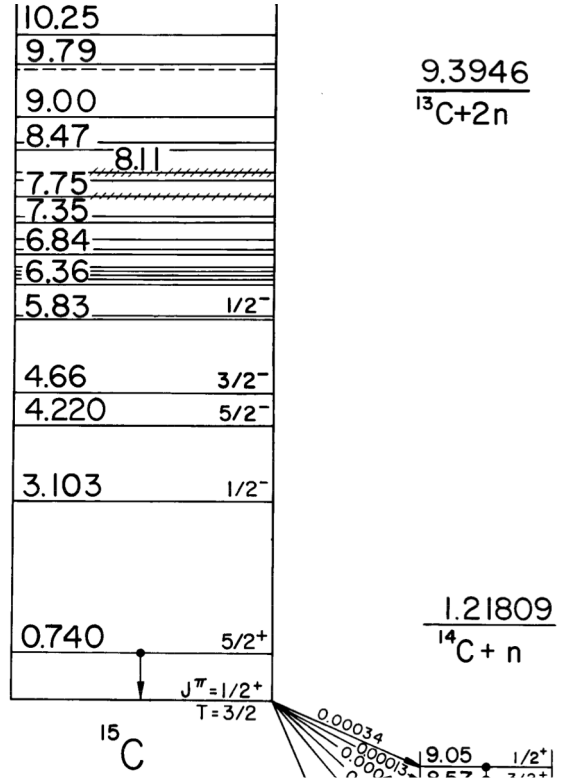
Angelo Calci,[1,*] Petr Navrátil,[1,†] Robert Roth,[2] Jérémy Dohet-Eraly,[1,‡] Sofia Quaglioni,[3] and Guillaume Hupin[4,5]

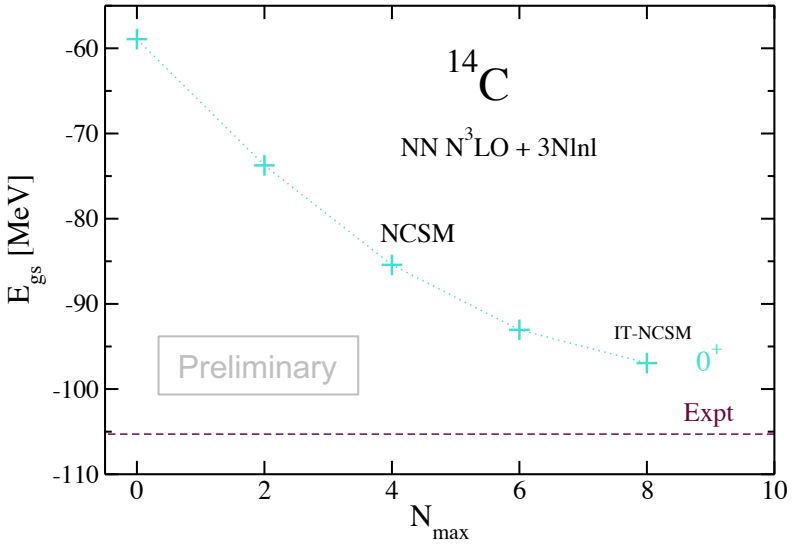
Halo *sd*-shell nucleus ^{15}C and its unbound mirror ^{15}F

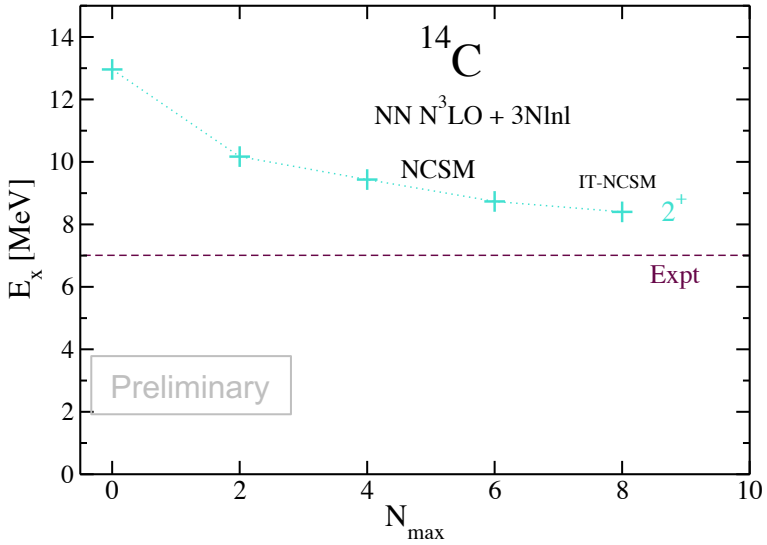
- Calculations in progress – all results preliminary
- Technical details
  - Step 1: **NN and 3N matrix elements**
- NN matrix elements – N^{3}LO Entem & Machleidt 2003, SRG evolved with λ = 2.0 fm^{-1}
  - ncsmv2b - Fortran90 with OpenMP
- 3N matrix elements – N^{2}LO with local/non-local regulator, SRG evolved with λ = 2.0 fm^{-1}
  - manyeff, v3trans – Fortran90 with OpenMP



Halo *sd*-shell nucleus ^{15}C

- Technical details
  - Step 2: **NCSM diagonalization – eigenvalues and wave functions**
- ncsd – Lanczosh algorithm, bit operations, hashing, partial or full storing of non-zero matrix elements in memory, Fortran 90 with MPI, ~12,000 MPI tasks
  - NN, NN+3N or NN+3N(NO2b) interactions
  - Calculations of N_{max} sequence (0(1),2(3),…N_{max})
  - Importance truncation

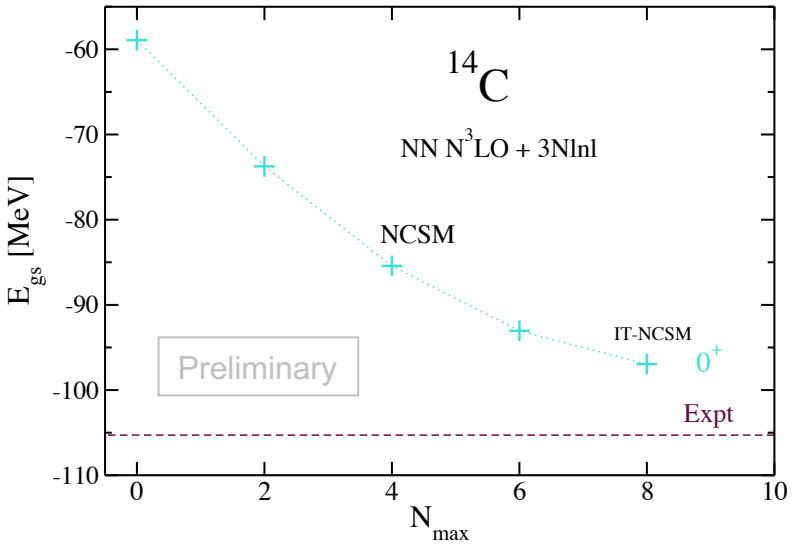


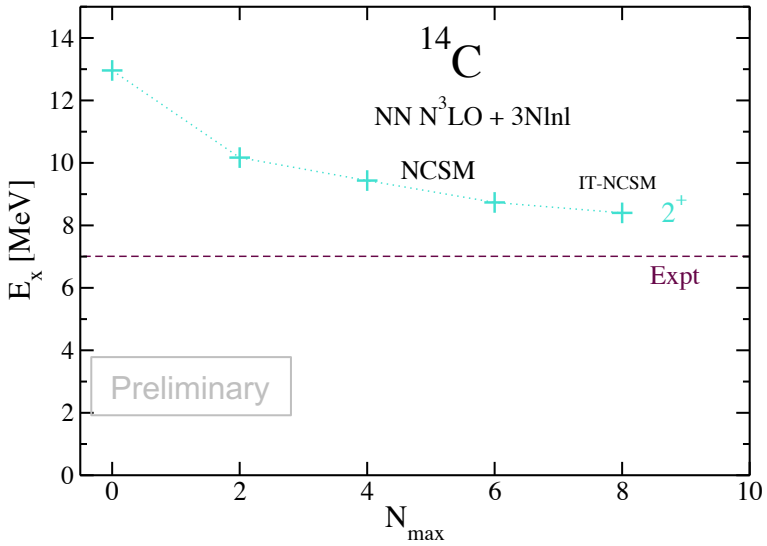


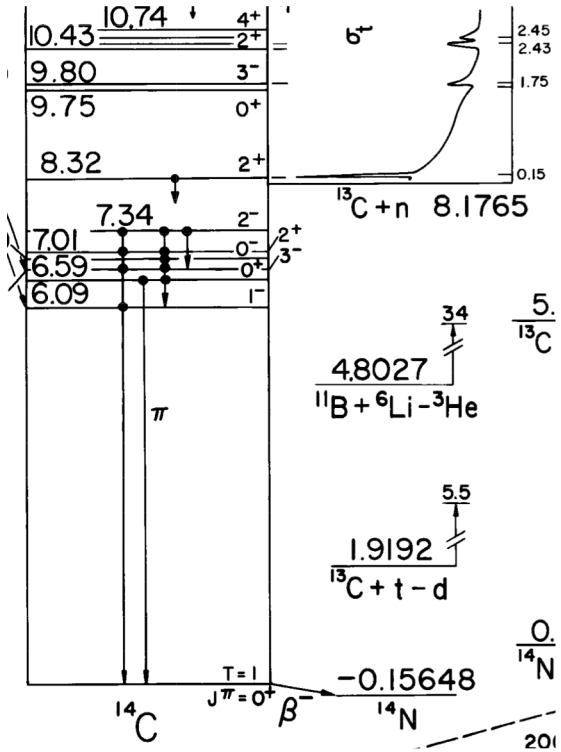
^{14}C ground state and 2$^+$ state
up to N_{max}=6 full space
(m-scheme dim=33,710,135)
Importance truncation in N_{max}=8
(largest m-scheme dim=46,126,926)
Complete 3N force (no normal ordering)
6144 MPI tasks with 16 GB/task
Titan@ORNL

Halo *sd*-shell nucleus ^{15}C

- Technical details
  - Step 2: **NCSM diagonalization – eigenvalues and wave functions**
- ncsd – Lanczosh algorithm, bit operations, hashing, partial or full storing of non-zero matrix elements in memory, Fortran 90 with MPI, ~12,000 MPI tasks
  - NN, NN+3N or NN+3N(NO2b) interactions
  - Calculations of N_{max} sequence (0(1),2(3),…N_{max})
  - Importance truncation







Halo *sd*-shell nucleus ^{15}C

- Technical details
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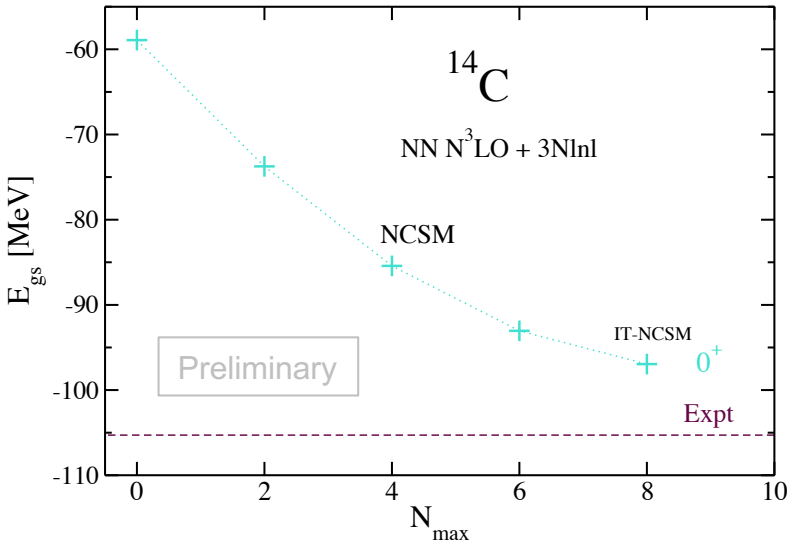
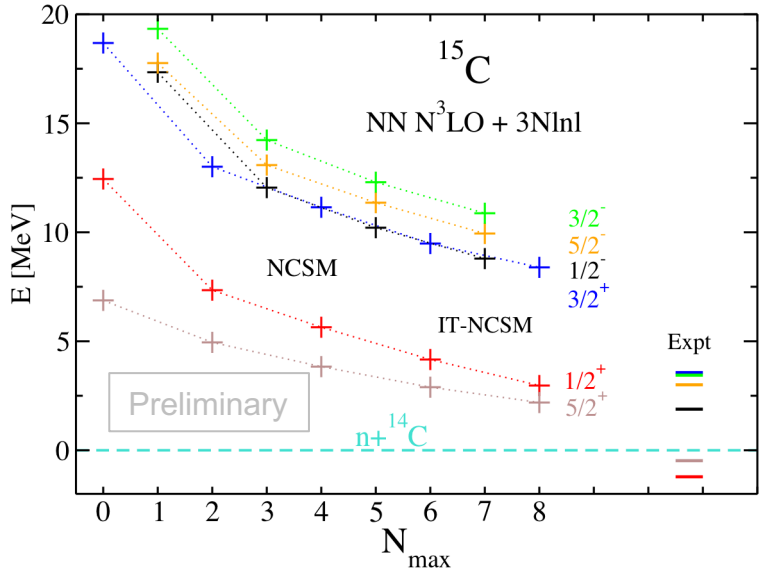
- ncsd – Lanczosh algorithm, bit operations, hashing, partial or full storing of non-zero matrix elements in memory, Fortran 90 with MPI, ~12,000 MPI tasks
  - NN, NN+3N or NN+3N(NO2b) interactions
  - Calculations of N_{max} sequence (0(1),2(3),…N_{max})
  - Importance truncation

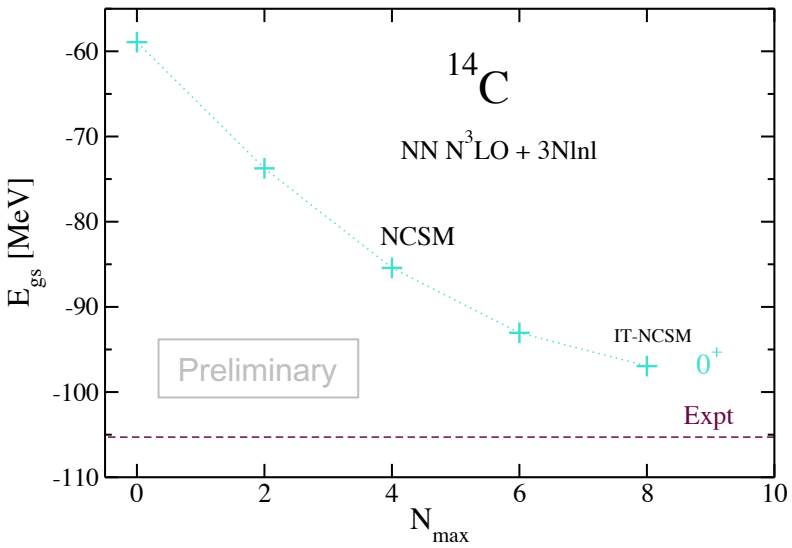


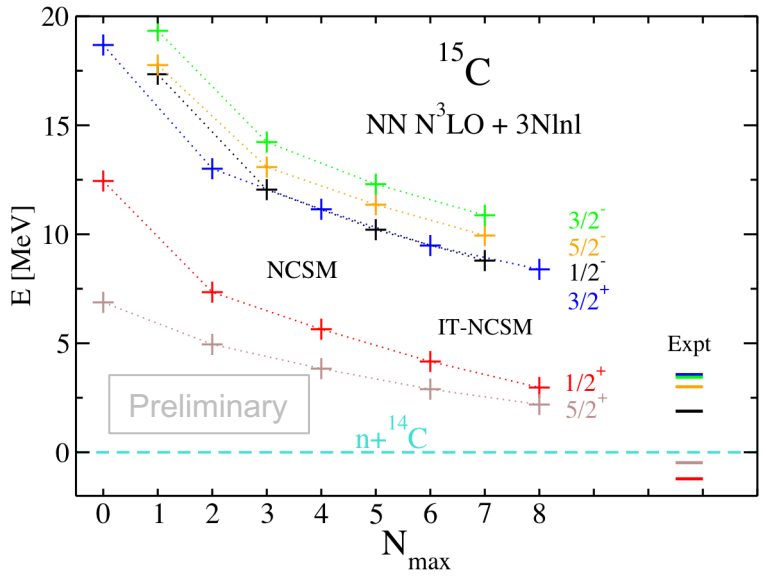


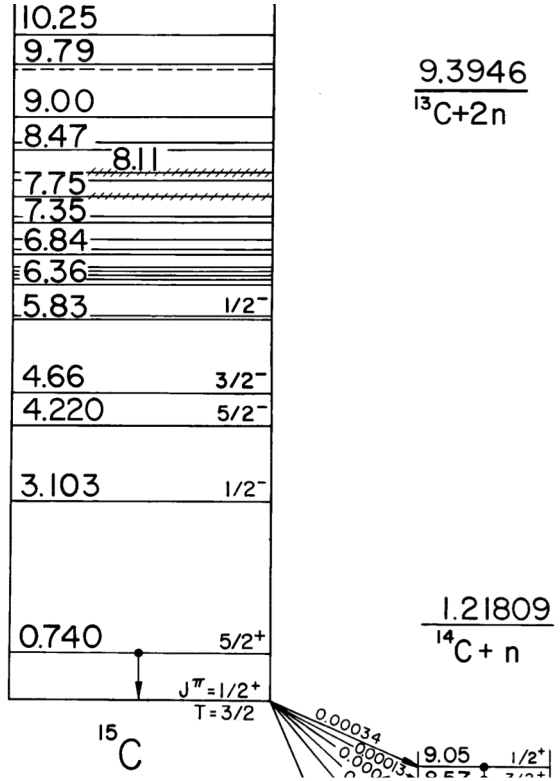
^{15}C positive and negative-parity states up to N_{max}=5 full space
(m-scheme dim=21,182,475)
Importance truncation in N_{max}=6,7,8
(largest m-scheme dim=105,023,779)
Complete 3N force (no normal ordering)
8192 MPI tasks with 16 GB/task
Titan@ORNL

Halo *sd*-shell nucleus ^{15}C

- Technical details
  - Step 2: **NCSM diagonalization – eigenvalues and wave functions**
- ncsd – Lanczosh algorithm, bit operations, hashing, partial or full storing of non-zero matrix elements in memory, Fortran 90 with MPI, ~12,000 MPI tasks
  - NN, NN+3N or NN+3N(NO2b) interactions
  - Calculations of N_{max} sequence (0(1),2(3),…N_{max})
  - Importance truncation

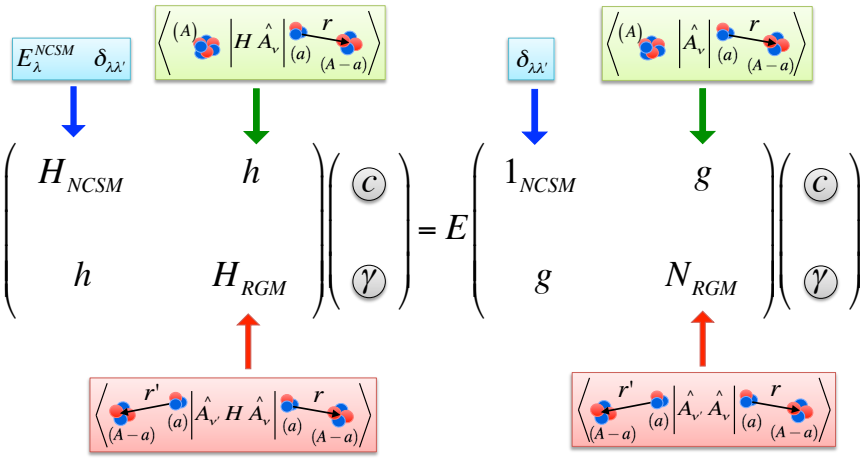




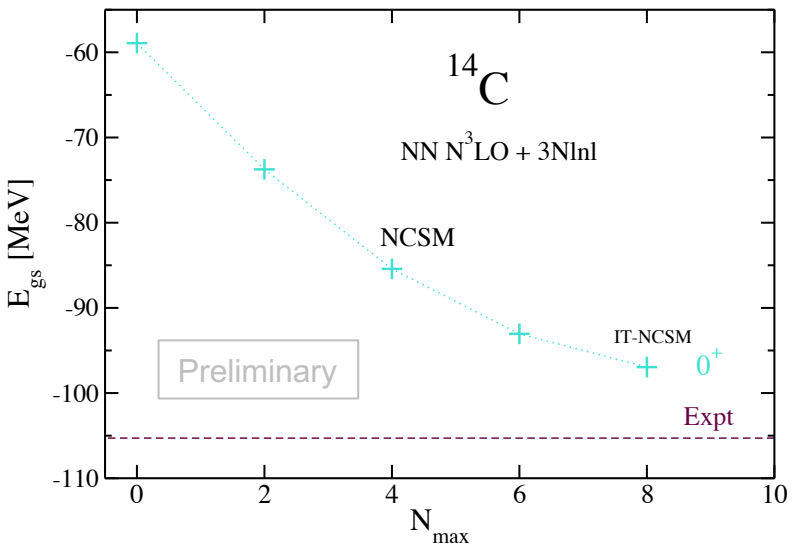


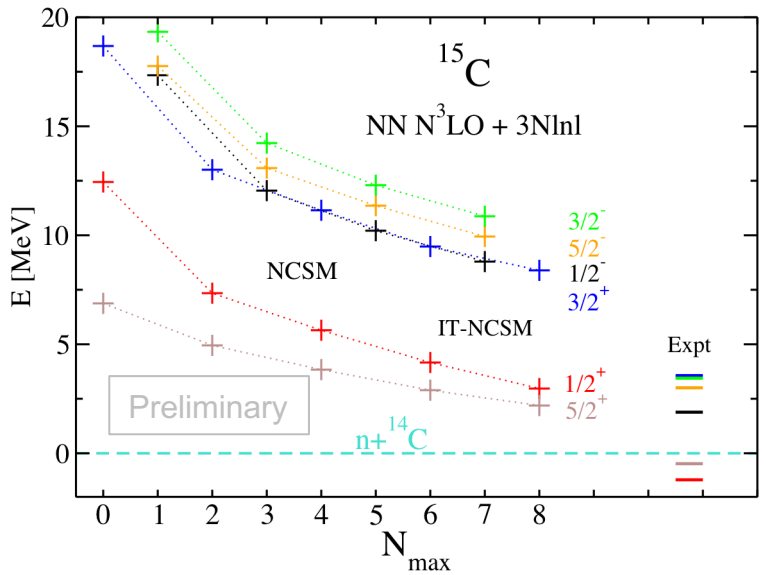
Halo *sd*-shell nucleus ^{15}C

- Technical details
  - Step 3: **RGM and coupling kernels**
- trdens code – bit operations, hashing, Fortran90 with MPI, ~16,000 MPI tasks
  - New algorithm



$$
\begin{aligned}
&{}_{\rm SD}\langle \Phi^{J^\pi T}_{\nu' n'} | \hat{P}_{A-1,A} \hat{V}^{\rm 3N}_{A-3\,A-2\,A-1} | \Phi^{J^\pi T}_{\nu n} \rangle_{\rm SD} \\
&= \frac{1}{6(A-1)(A-2)(A-3)} \sum_{jj'} \hat{s}\hat{s}'\hat{j}\hat{j}' \\
&\times (-1)^{2J+I_1+I_1'+j+j'} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ \ell & J & j \end{Bmatrix} \begin{Bmatrix} I_1' & \frac{1}{2} & s' \\ \ell' & J & j' \end{Bmatrix} \\
&\times \sum_{M_1 m_j M_{T_1} m_t M_1' m_j' M_{T_1}' m_t'} \\
&\times C^{JM_J}_{I_1 M_1 j m_j} C^{TM_T}_{T_1 M_{T_1} \frac{1}{2} m_t} C^{JM_J'}_{I_1' M_1' j' m_j'} C^{TM_T'}_{T_1' M_{T_1}' j' m_t'} \\
&\times \sum_{abdef} \langle ab\ n'\ell'j'm_j'\tfrac{1}{2}m_t' | \hat{V}^{\rm 3N} | def \rangle \\
&\times {}_{\rm SD}\langle A-1\ \alpha_1' I_1'^{\pi_1'} M_1' T_1' M_{T_1}' | \hat{a}^\dagger_{n\ell j m_j \frac{1}{2} m_t} \\
&\times \hat{a}_b^\dagger \hat{a}_a^\dagger \hat{a}_d \hat{a}_e \hat{a}_f \ | A-1\ \alpha_1 I_1^{\pi_1} M_1 T_1 M_{T_1} \rangle_{\rm SD},
\end{aligned}
$$

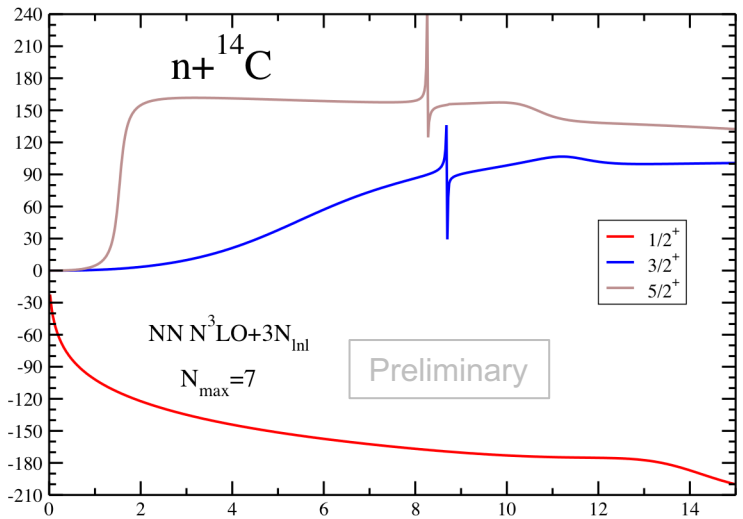


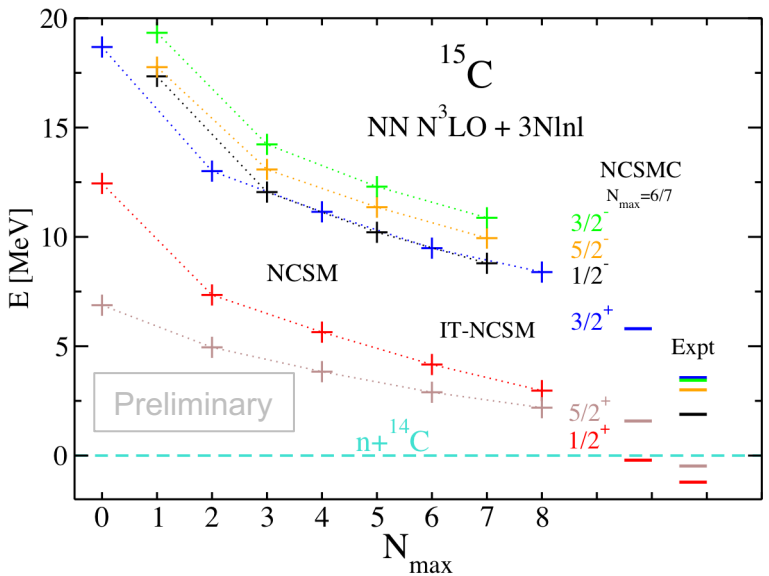


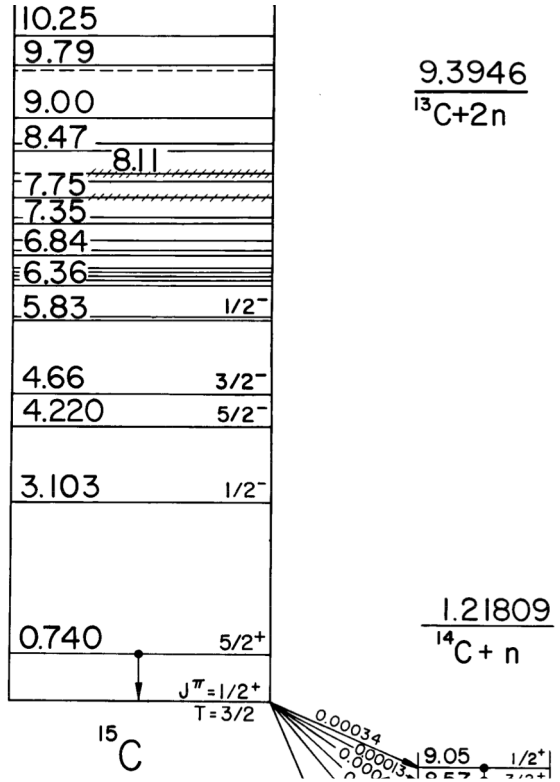
RGM and coupling kernels calculated for N_{max}=6/7
Complete 3N force (no normal ordering)
RGM kernels - ^{14}C 0^+, 2^+ - 25 contributions
16384 MPI tasks with 4 GB/task
Titan@ORNL
Coupling kernels -^{14}C 0^+, 2^+ - 5 contributions
1024 MPI tasks on Eos@ORNL

Halo *sd*-shell nucleus ^{15}C

- Technical details
  - Step 4: **NCSMC calculation**
- ncsmc – Fortran90 with OpenMP and MPI
  - RGM and coupling kernels either input or calculated from densities
  - Solves NCSMC coupled equations, calculates the S-matrix and scattering/reaction observables







Halo *sd*-shell nucleus ^{15}C

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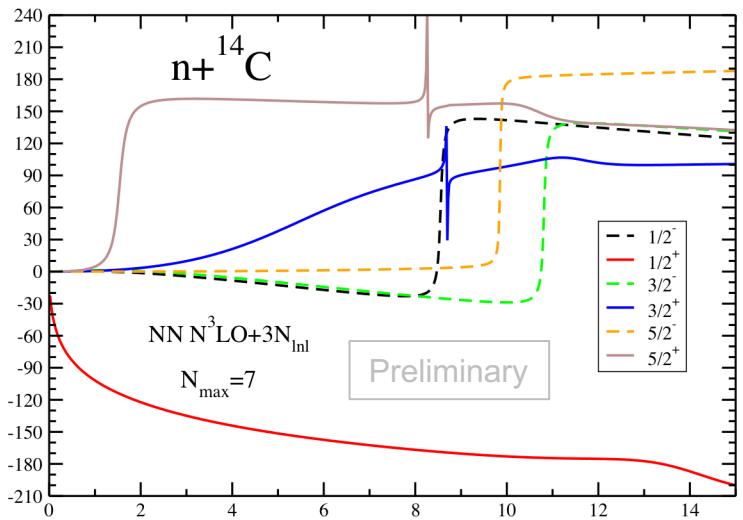

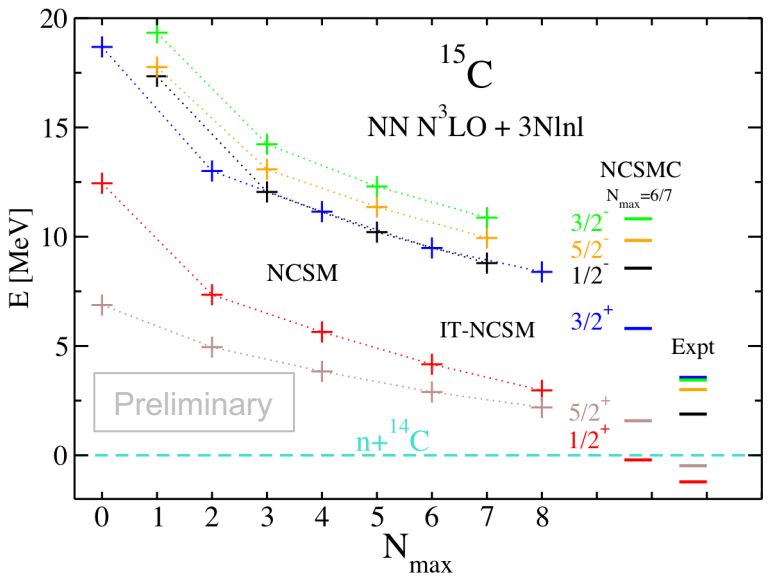

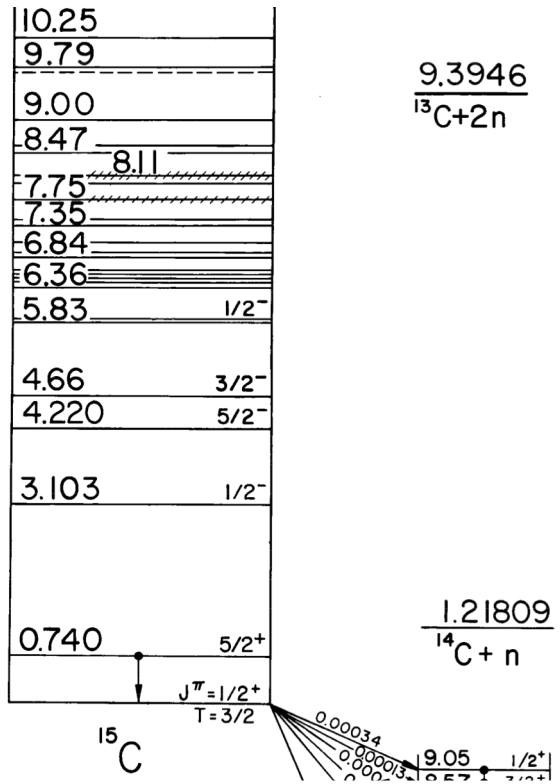

Halo *sd*-shell nucleus ^{15}C

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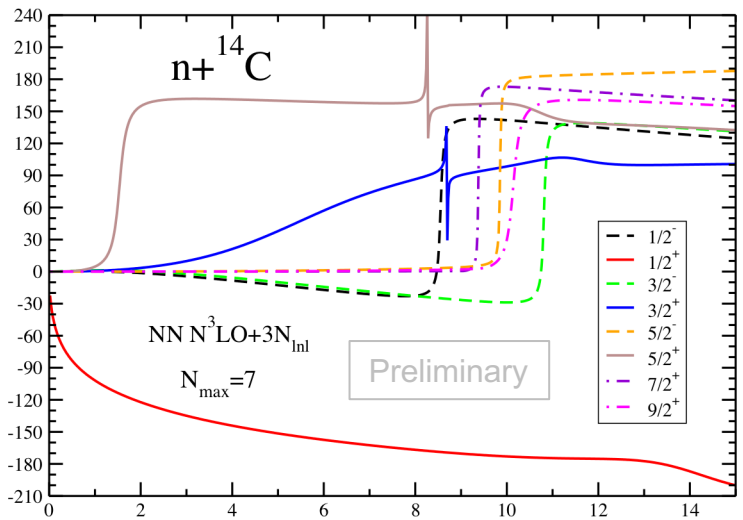

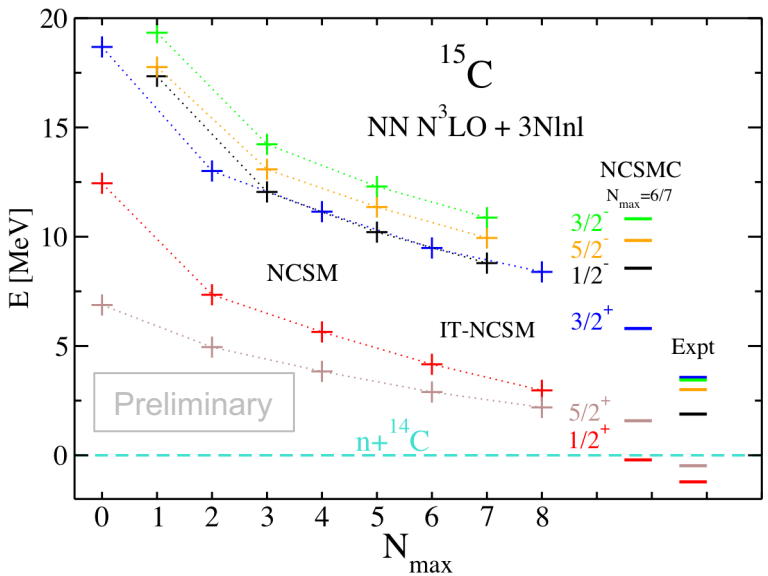

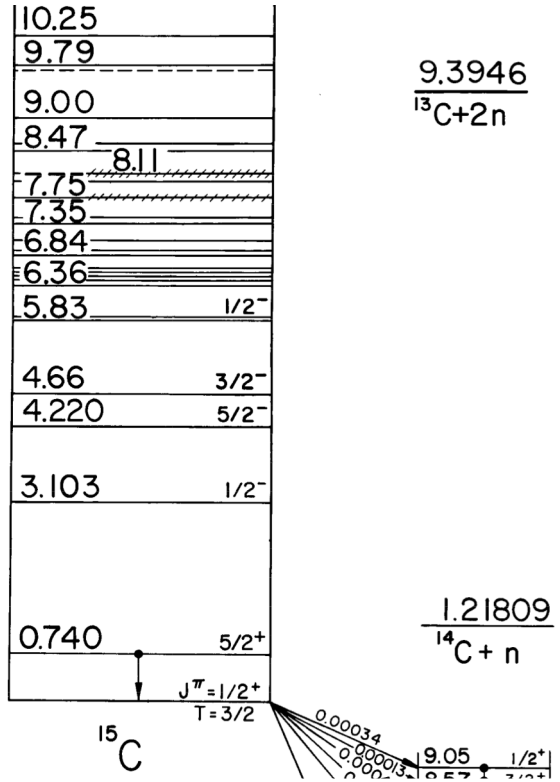

Halo *sd*-shell nucleus ^{15}C

- Technical details
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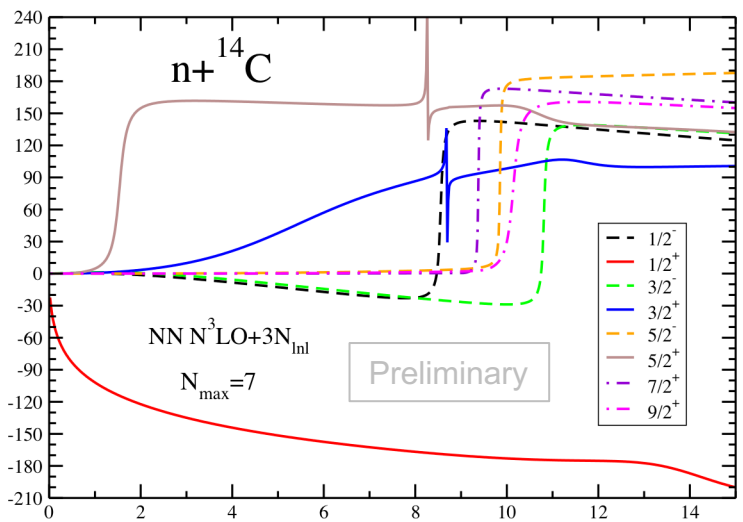

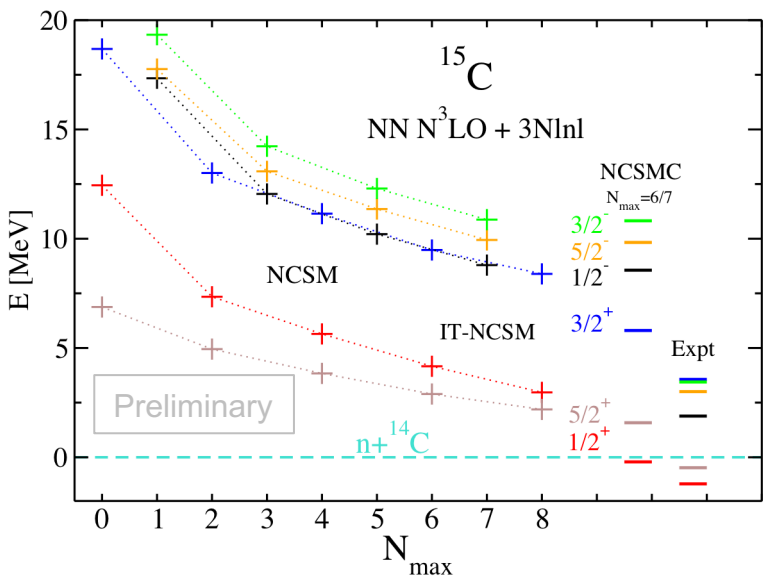

Table 15.1 from (1991AJ01): Energy levels of ^{15}C [a]

E_x (MeV ± keV)	$J^\pi; T$	τ or $\Gamma_{c.m.}$ (keV)	Decay	Reactions
g.s.	$\frac{1}{2}^+; \frac{3}{2}$	$\tau_{1/2} = 2.449 \pm 0.005$ s	β^-	1, 2, 3, 4, 6, 7, 9
		$\lvert g\rvert = 2.63 \pm 0.14$		
0.7400 ± 1.5	$\frac{5}{2}^+$	$\tau_m = 3.76 \pm 0.10$ ns	γ	2, 3, 4, 7, 8
		$g = -0.703 \pm 0.012$		
3.103 ± 4	$\frac{1}{2}^-$	$\Gamma_{c.m.} \leq 40$		2, 3, 9
4.220 ± 3	$\frac{5}{2}^-$	< 14		2, 3
4.657 ± 9	$\frac{3}{2}^-$			2, 3
4.78 ± 100	$\frac{3}{2}^+$	1740 ± 400		6
5.833 ± 20	$(\frac{3}{2}^+)$	64 ± 8		2, 6
5.866 ± 8	$\frac{1}{2}^-$			2, 3
6.358 ± 6	$(\frac{5}{2}, \frac{7}{2}^+, \frac{9}{2}^+)$	< 20		2, 3
6.417 ± 6	$(\frac{3}{2} \to \frac{7}{2})$	≈ 50		2, 3
6.449 ± 7	$(\frac{9}{2}^-, \frac{11}{2})$	< 14		2, 3
6.536 ± 4	[a]	< 14		2, 3
6.626 ± 8	$(\frac{3}{2})$	20 ± 10		2, 3
6.841 ± 4	[a]	< 14		2, 3
6.881 ± 4	$(\frac{9}{2})$ [a]	< 20		2, 3
7.095 ± 4	$(\frac{3}{2})$	< 15		2, 3
7.352 ± 6	$(\frac{9}{2}, \frac{11}{2})$	20 ± 10		2, 4
7.414 ± 20				2
7.75 ± 30 [b]				2
8.01 ± 30				2

Conclusions

- *Ab initio* calculations of nuclear structure and reactions with predictive power becoming feasible beyond the lightest nuclei
- These calculations make connections between the low-energy QCD, many-body systems, and nuclear astrophysics
- ^{15}C NCSMC calculations in progress
  - Capture cross section, cluster form factor, ANCs
- Study of the unbound ^{15}F (mirror of ^{15}C) in progress
  - Structure of resonances

TRIUMF

Thank you!
Merci!
ありがとうございました

Discovery, accelerated