Applications of the *Ab Initio* No-Core Shell Model

Celebrating 75 Years of the Nuclear Shell Model and Maria Goeppert-Mayer

ANL, July 19-21, 2024

Petr Navratil

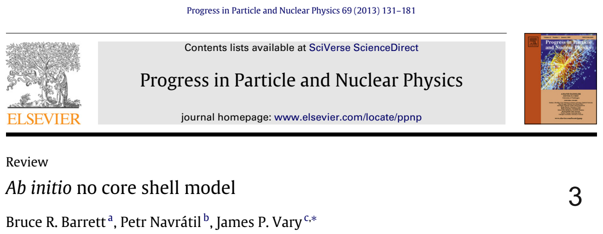
TRIUMF

Outline

- Introduction – Shell Model vs. No-Core Shell Model
- *Ab initio* nuclear theory – no-core shell model (NCSM)
- Early NCSM applications - Okubo – Lee – Suzuki (OLS) renormalization
- Recent NCSM applications - Similarity Renormalization Group (SRG) renormalization
- No-Core Shell Model with Continuum (NCSMC) - Unified description of bound and unbound states
- Conclusions

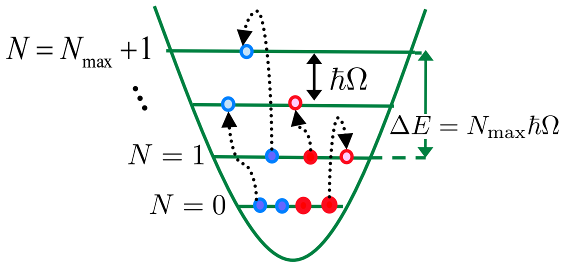
Shell Model

No-Core Shell Model (NCSM)



Solving many-nucleon Schroedinger equation

$$H\psi_n = E_n\psi_n$$

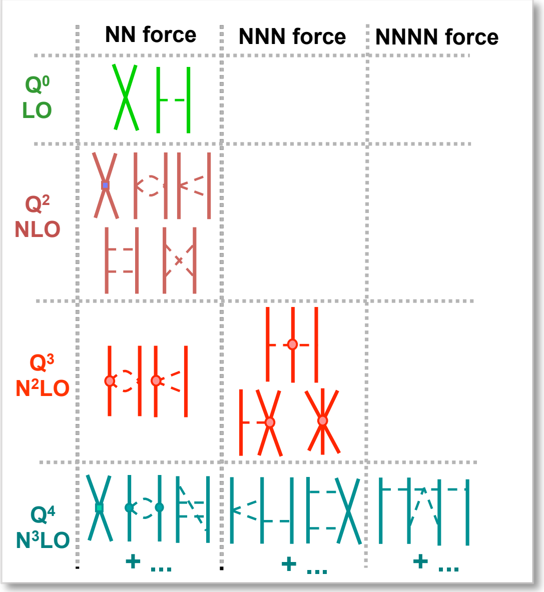


Basis expansion method

Shell Model	NCSM
Harmonic oscillator (HO) or other Slater determinant (SD) basis	Relative-coordinate or SD HO basis truncated with N_{max}
Single shell valence space	Many HO shells

Interaction

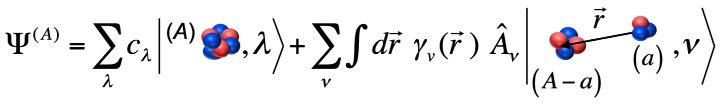
Shell Model	NCSM
Effective NN interaction fitted to many-nucleon data – CK, USD, KB3…	Chiral NN+3N interaction fitted to few-body systems (*NN*, A=3,4) - bare or renormalized by SRG (earlier work - Okubo-Lee-Suzuki)



Predicts nuclear structure properties of nuclei

Shell Model	NCSM
Across nuclear chart	Light nuclei (A≤20)

Extendable to describe scattering & reactions – NCSM with continuum



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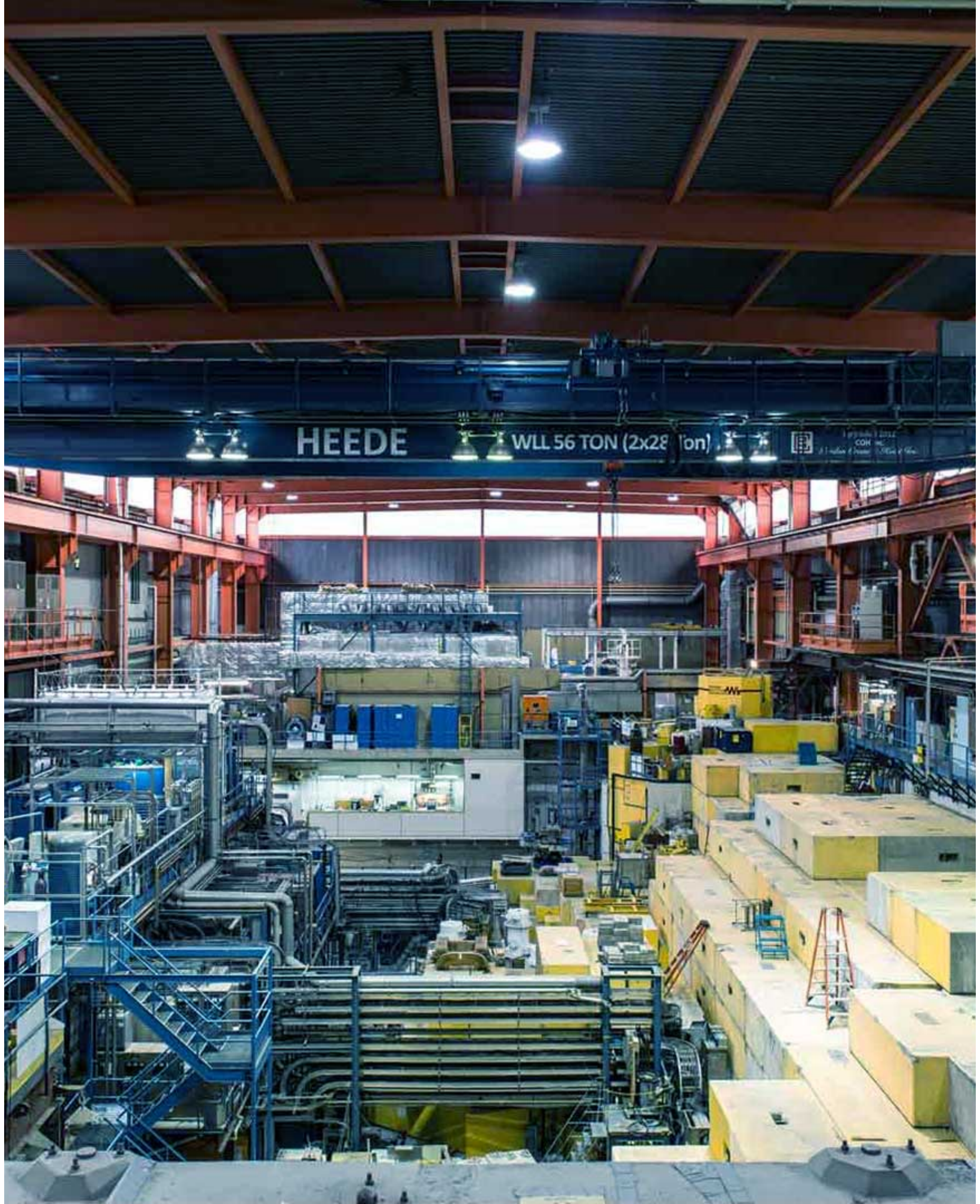
Ab initio nuclear theory - no-core shell model (NCSM)



Discovery, accelerated

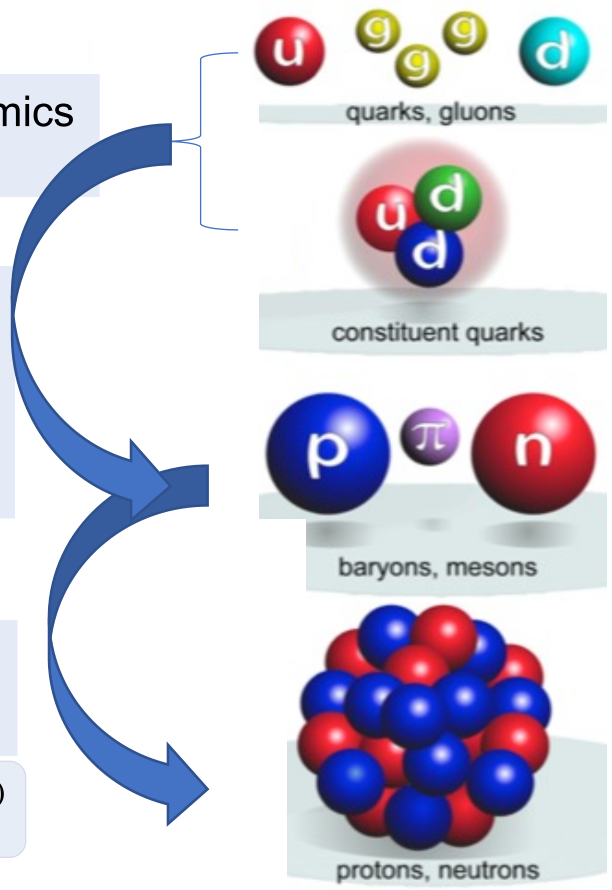
First principles or *ab initio* nuclear theory

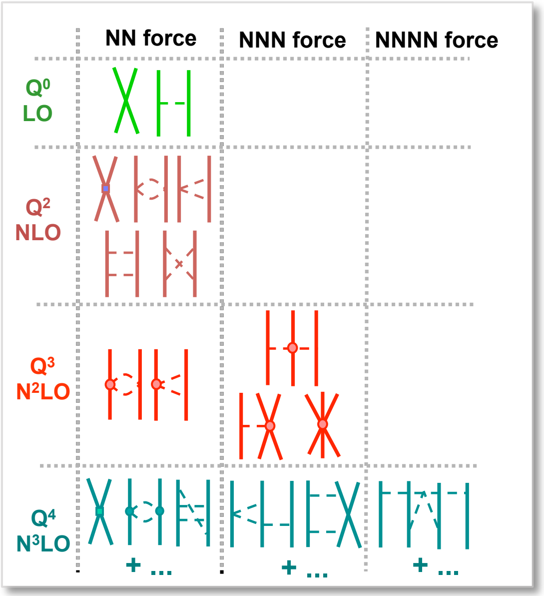
Quantum Chromodynamics (QCD)

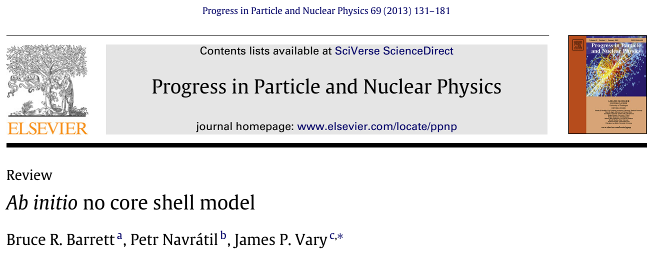
Chiral Effective Field Theory (parameters fitted to NN data)

Current *ab initio* nuclear theory

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






Progress in Particle and Nuclear Physics 69 (2013) 131–181
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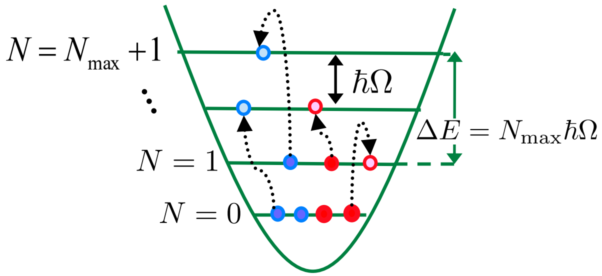
Contents lists available at SciVerse ScienceDirect
Progress in Particle and Nuclear Physics
journal homepage: www.elsevier.com/locate/ppnp
Review
Ab initio no core shell model
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

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

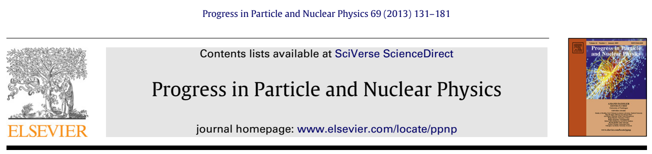
NCSM

- 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(Jacobi)-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



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

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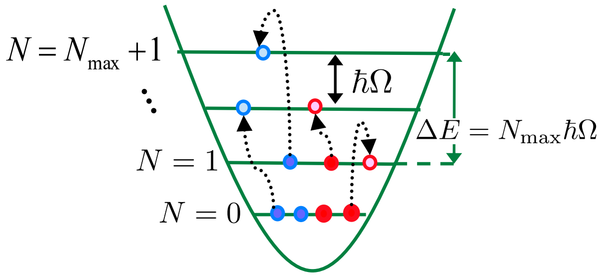

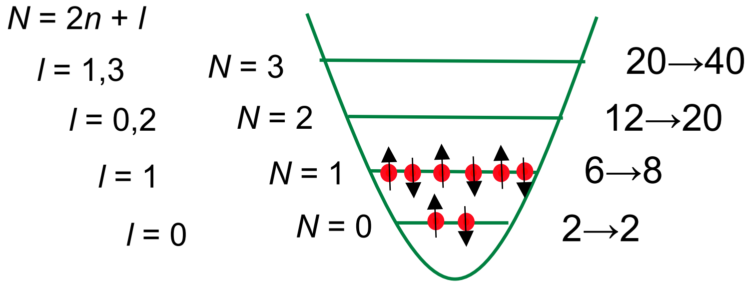

$$E = (2n + l + \tfrac{3}{2})\hbar\Omega$$

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

$$\Psi_{SD}^A = \sum_{N=0}^{N_{max}} \sum_j c_{Nj}^{SD} \Phi_{SD\,Nj}^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{CM})$$

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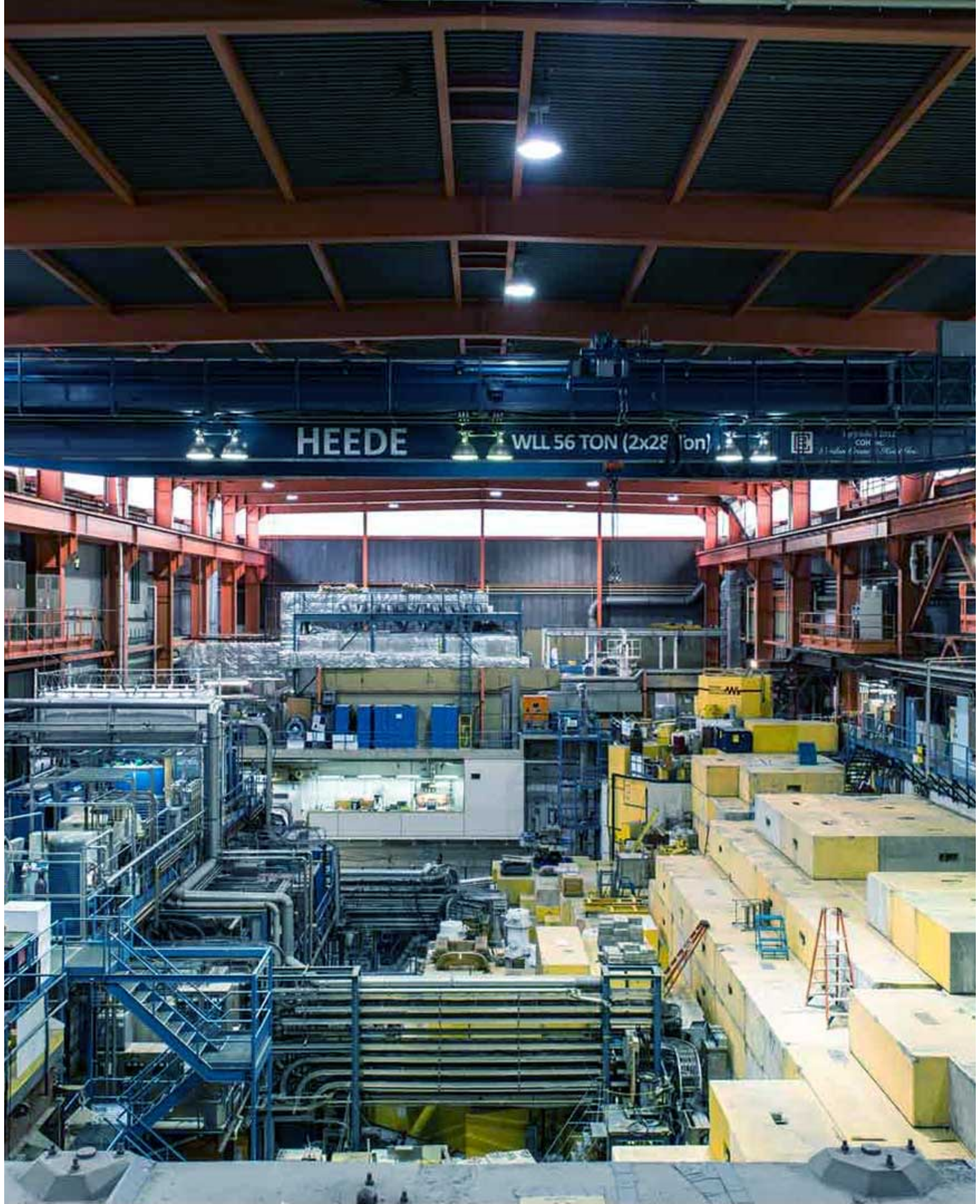
Early NCSM applications - Okubo – Lee – Suzuki (OLS) renormalization (calculations not variational)



Discovery, accelerated

NCSM early developments

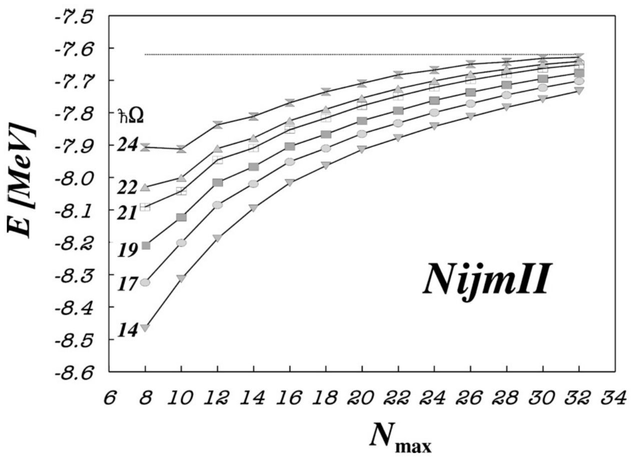
- Confirmation that NCSM calculations of the ^{3}H gs energy reproduce Faddeev method results
- Later, the NCSM ^{4}He gs energy prediction with the CD-Bonn potential was confirmed by Faddeev-Yakubovsky calculations

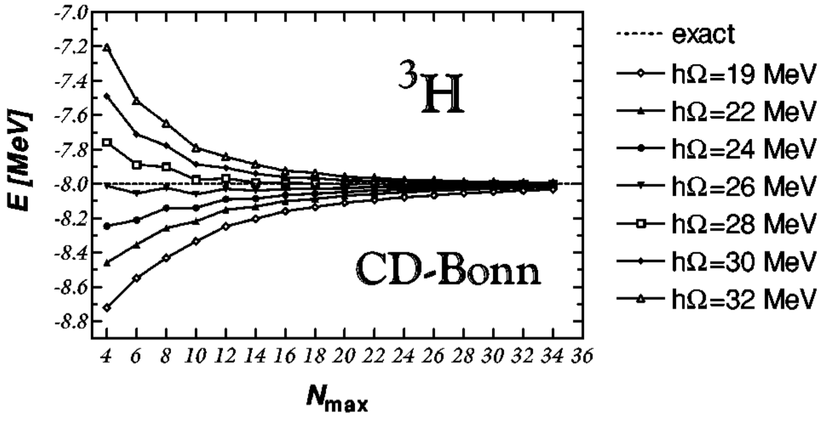
  - Jacobi-coordinate HO basis
  - Okubo-Lee-Suzuki effective interaction

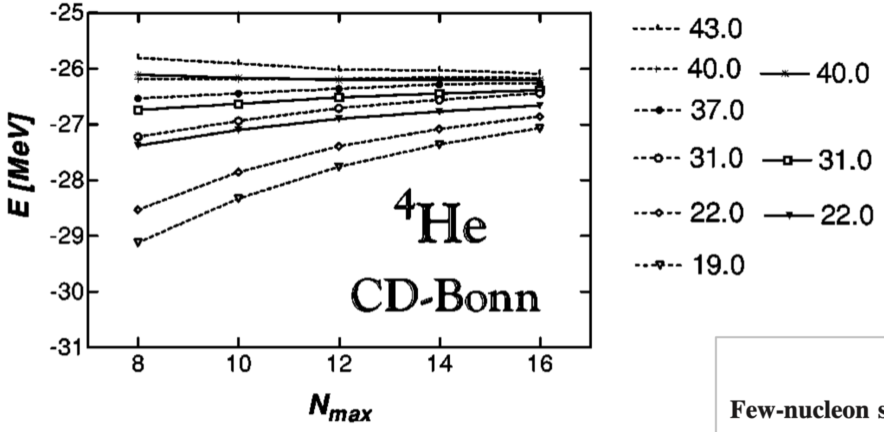
PHYSICAL REVIEW C VOLUME 57, NUMBER 2 FEBRUARY 1998

Shell-model calculations for the three-nucleon system

P. Navrátil* and B. R. Barrett
Department of Physics, University of Arizona, Tucson, Arizona 85721
(Received 21 May 1997)







NCSM is
an *ab initio*
method

PHYSICAL REVIEW C, VOLUME 61, 044001

Few-nucleon systems in a translationally invariant harmonic oscillator basis

P. Navrátil,[1,2] G. P. Kamuntavičius,[1,3,4] and B. R. Barrett[1]

NCSM early developments

- Structure of ^{12}C
  - Energies of states and other properties of a complex nucleus can be predicted from an *ab initio* approach
  - Slater-Determinant HO basis
  - Okubo-Lee-Suzuki effective interaction

VOLUME 84, NUMBER 25 PHYSICAL REVIEW LETTERS 19 JUNE 2000

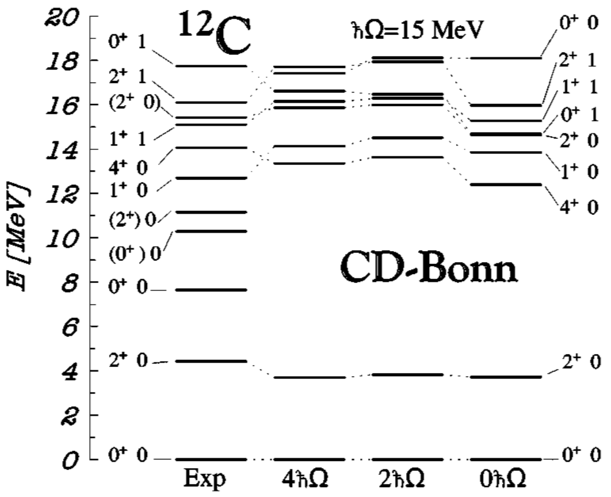
Properties of ^{12}C in the *Ab Initio* Nuclear Shell Model

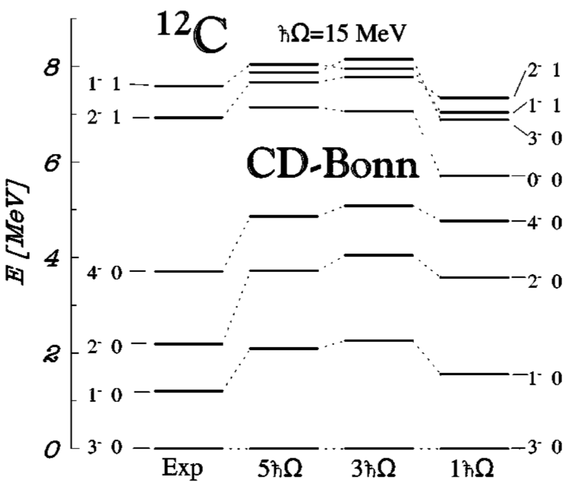
P. Navrátil,[1,2] J.P. Vary,[3] and B.R. Barrett[1]

PHYSICAL REVIEW C, VOLUME 62, 054311

Large-basis *ab initio* no-core shell model and its application to ^{12}C

P. Navrátil,[1,2,*] J. P. Vary,[3] and B. R. Barrett[1]

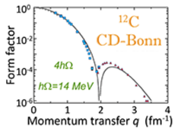




Physical Review C 50th Anniversary Milestones

PHYSICAL REVIEW C

This year, 2020, is the 50th anniversary of *Physical Review C*, which evolved from a section of its parent journal, *The Physical Review*, to one of the most read and trusted journals for nuclear physics. As part of the anniversary celebration, we are putting together a collection of milestone papers that remain central to developments in the field of nuclear physics. These papers announce major discoveries or open up new avenues of research. They would not have come to our journal, had the community not trusted and upheld the top-shelf quality of what PRC has traditionally published and intends to publish in the future.



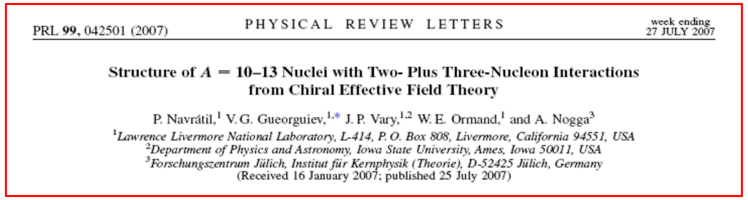
Large-basis *ab initio* no-core shell model and its application to ^{12}C

Coupled-cluster and configuration-interaction shell model methods originated decades ago. Today, by employing high-precision interactions, new conceptual tools, and powerful computers, these *ab initio* methods have shown the ability to compute energies and other observables, such as electron scattering form factors, for a wide range of atomic nuclei without adjustable parameters. These two papers were early demonstrations of the power of the revitalized methods.

Large-basis *ab initio* no-core shell model and its application to ^{12}C
P. Navrátil, J. P. Vary, and B. R. Barrett
Phys. Rev. C **62**, 054311 (2000)

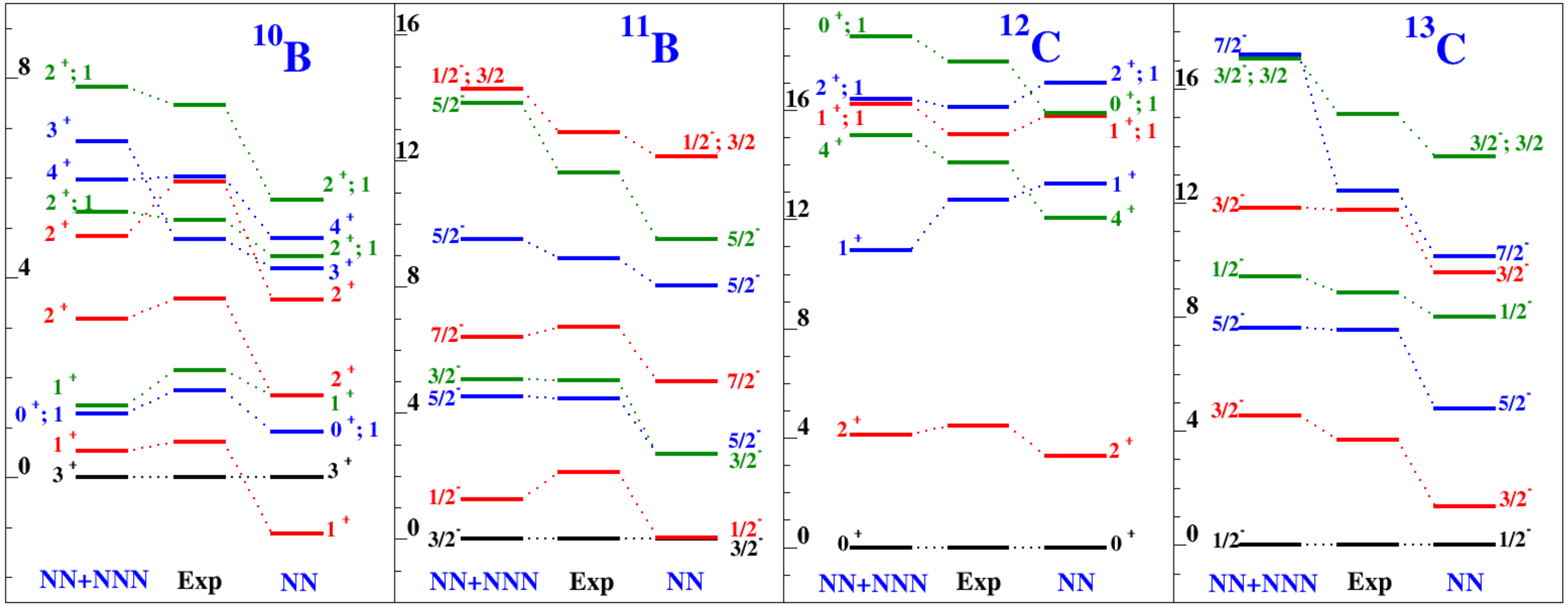
Structure of mid-*p*-shell nuclei with chiral NN+3N interactions

- 3N interaction essential to describe structure of nuclei
  - Both binding energies and excitation levels


PRL 99, 042501 (2007) PHYSICAL REVIEW LETTERS week ending 27 JULY 2007

Structure of $A = 10$–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]
[1]Lawrence Livermore National Laboratory, L-414, P. O. Box 808, Livermore, California 94551, USA
[2]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA
[3]Forschungszentrum Jülich, Institut für Kernphysik (Theorie), D-52425 Jülich, Germany
(Received 16 January 2007; published 25 July 2007)



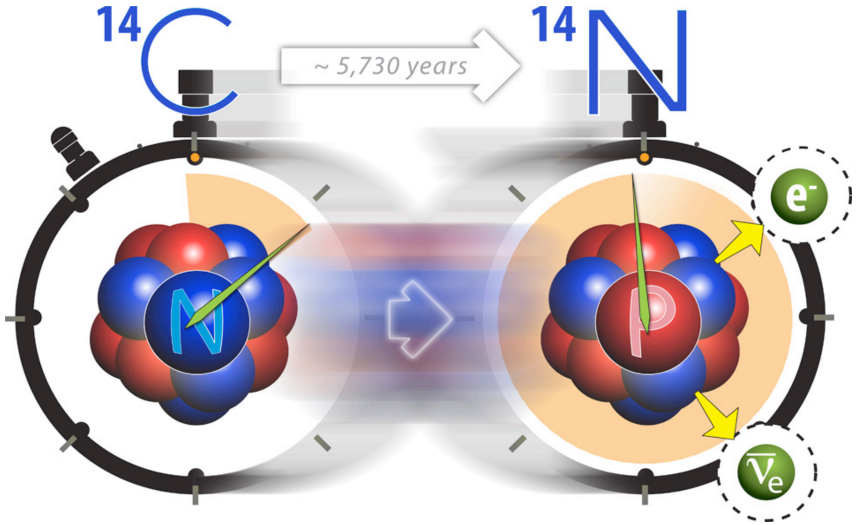
“Anomalous Long Lifetime of Carbon-14”

Objectives

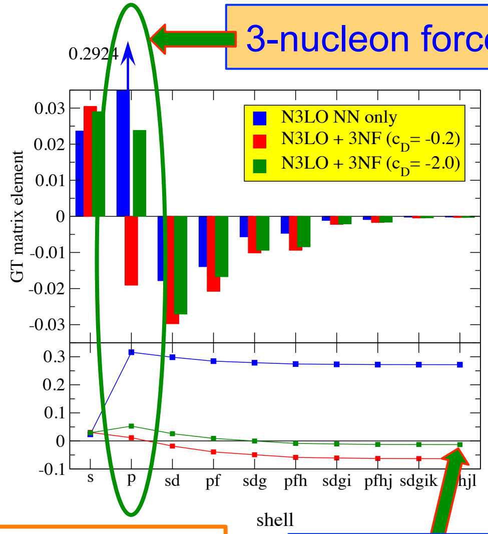
- Solve the puzzle of the long but useful lifetime of ^{14}C
- Determine the microscopic origin of the suppressed β-decay rate

Impact

- Establishes a major role for strong 3-nucleon forces in nuclei
- Verifies accuracy of *ab initio* microscopic nuclear theory
- Provides foundation for guiding DOE-supported experiments

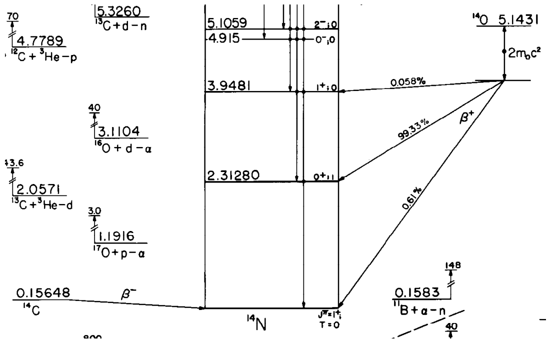


3-nucleon forces suppress critical component



net decay rate
Is very small

- Dimension of matrix solved for 8 lowest states ~ $1\text{x}10^9$
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- “Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)



^{14}N experiment

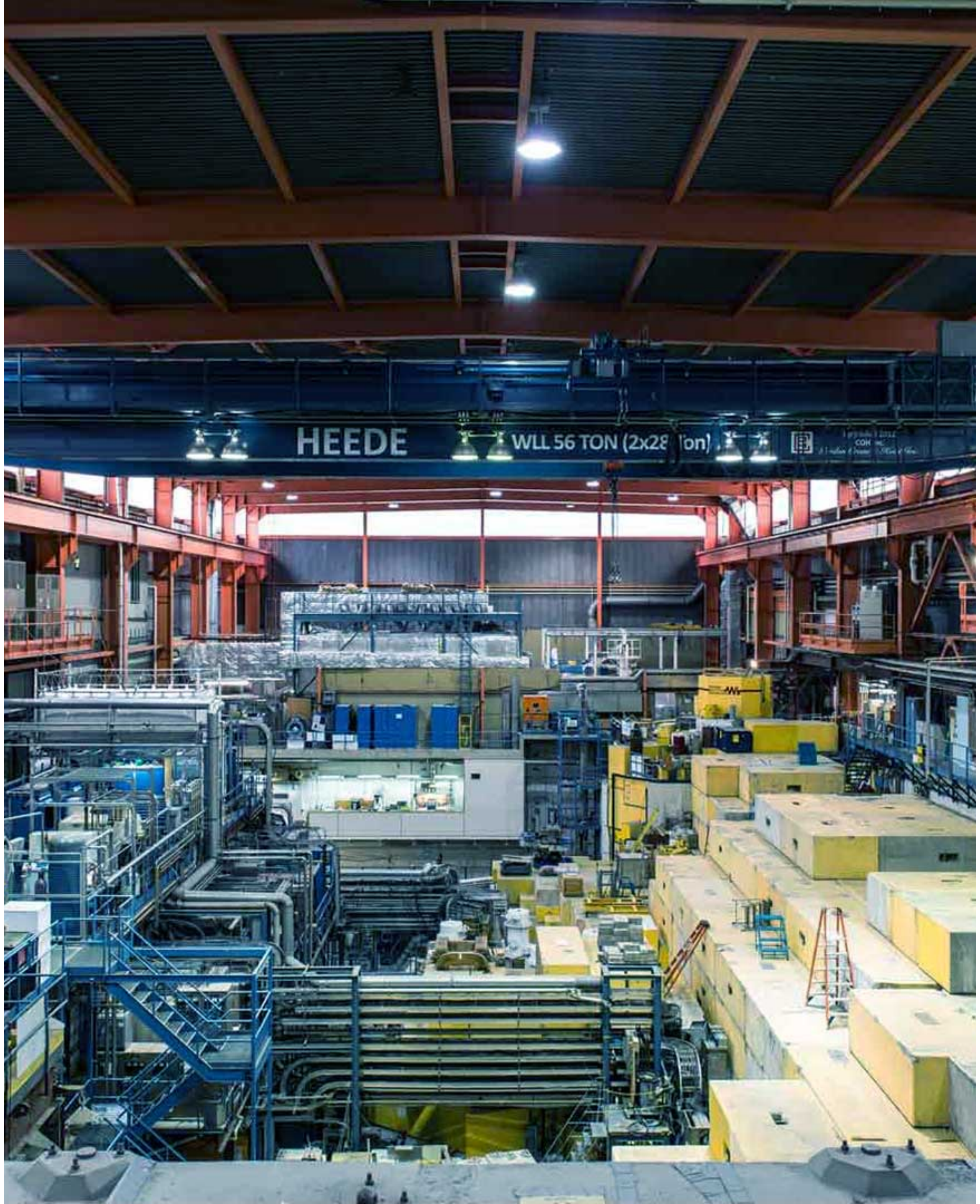
PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

P. Maris,[1] J. P. Vary,[1] P. Navrátil,[2,3] W. E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

TRIUMF

Recent NCSM applications - Similarity Renormalization Group (SRG) renormalization (variational calculations)



Discovery, accelerated

PHYSICAL REVIEW C **101**, 014318 (2020)

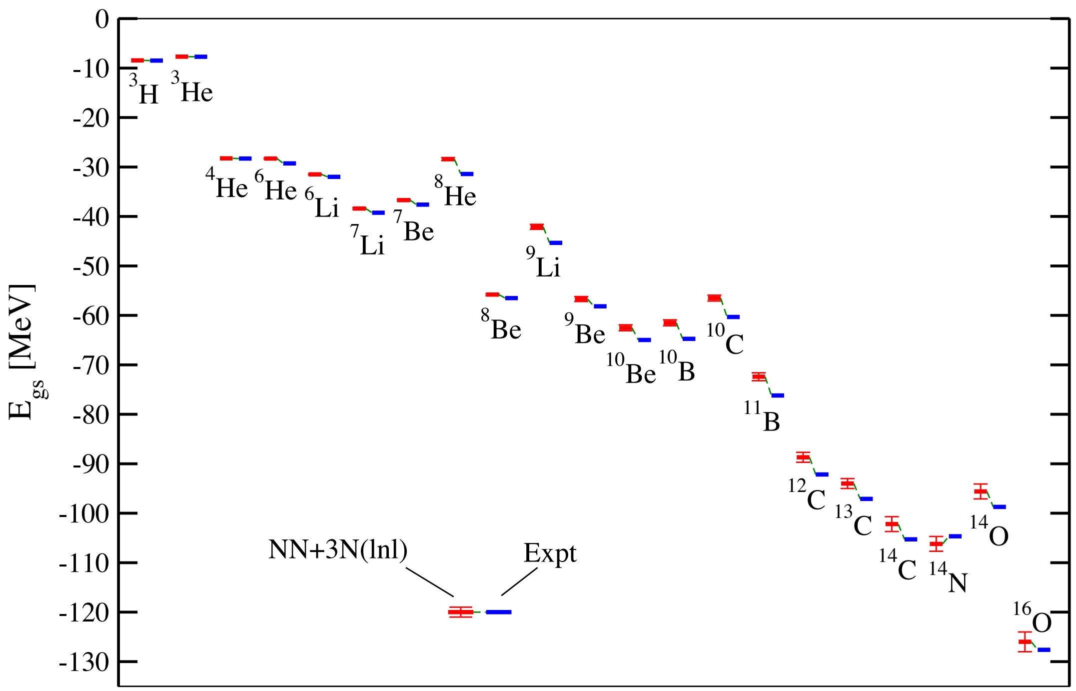
Novel chiral Hamiltonian and observables in light and medium-mass nuclei

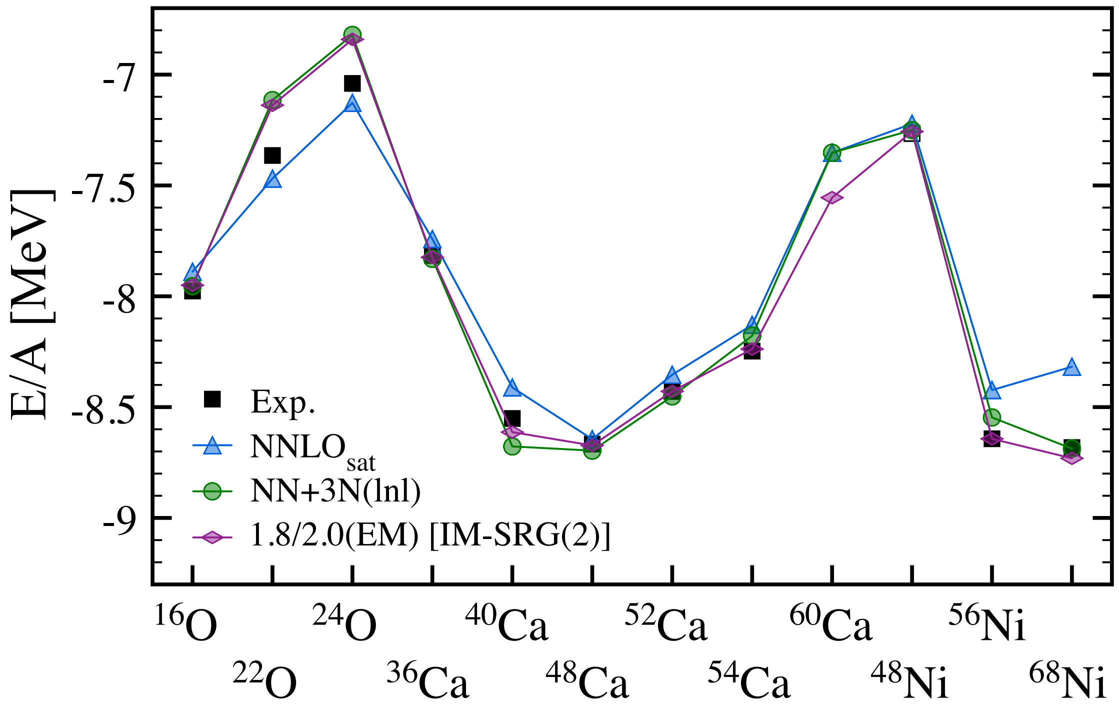
V. Somà,[1,*] P. Navrátil,[2,†] F. Raimondi,[3,4,‡] C. Barbieri,[4,§] and T. Duguet[1,5,‖]

Binding energies of atomic nuclei with NN+3N forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
  - **The Hamiltonian fully determined in *A*=2 and *A*=3,4 systems**
    - Nucleon–nucleon scattering, deuteron properties, ^{3}H and ^{4}He binding energy, ^{3}H half life
  - Light nuclei – NCSM
  - Medium mass nuclei – Self-Consistent Green's Function method

NN N^{3}LO (Entem-Machleidt 2003)
3N N^{2}LO w local/non-local regulator





1.8/2.0 (EM) results: J. Simonis, S. R. Stroberg, K. Hebeler, J. D. Holt, and A. Schwenk, Phys. Rev. C 96, 014303 (2017).

PHYSICAL REVIEW C **101**, 014318 (2020)

Novel chiral Hamiltonian and observables in light and medium-mass nuclei

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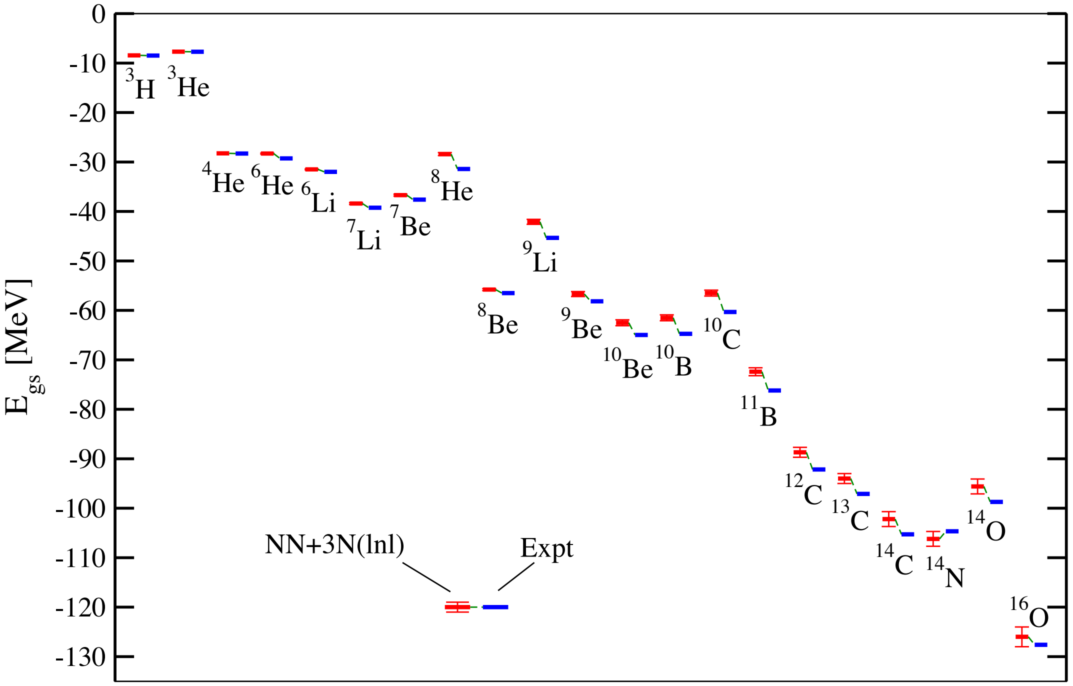
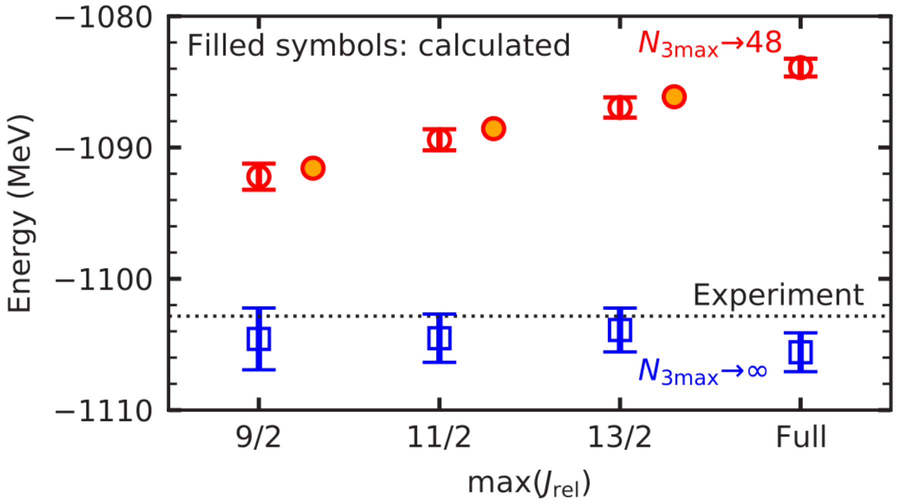
NN N^{3}LO (Entem-Machleidt 2003)
3N N^{2}LO w local/non-local regulator



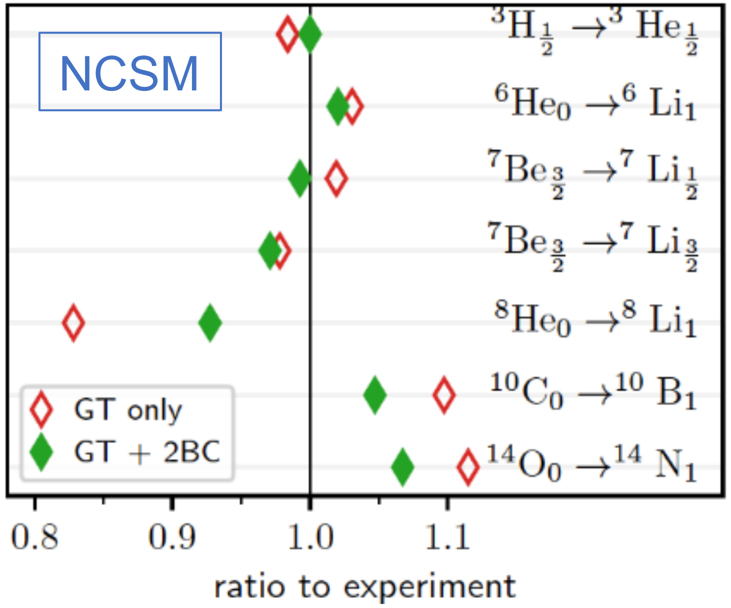


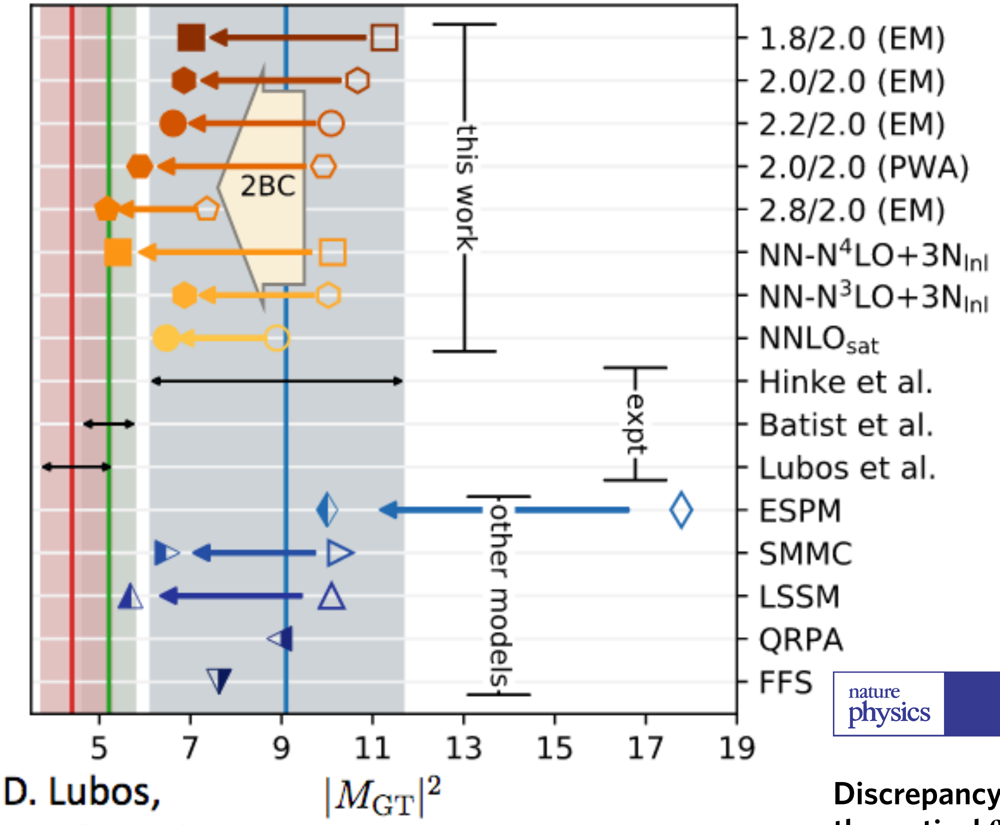
PHYSICAL REVIEW C **105**, 014302 (2022)

Converged *ab initio* calculations of heavy nuclei

T. Miyagi,[1,*] S. R. Stroberg,[2,†] P. Navrátil,[1,‡] K. Hebeler,[3,4,5,§] and J. D. Holt[1,6,||]

50-year-old puzzle of quenched beta decays resolved from first principles

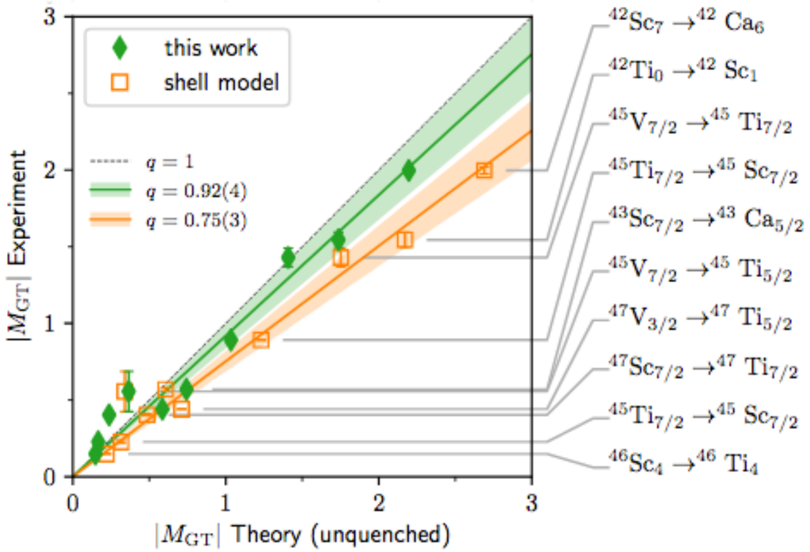




D. Lubos, PRL (2019)

$^{100}Sn \to ^{100}In$

The strongest Gamow–Teller strength so far measured in all atomic nuclei



nature physics LETTERS
https://doi.org/10.1038/s41567-019-0450-7

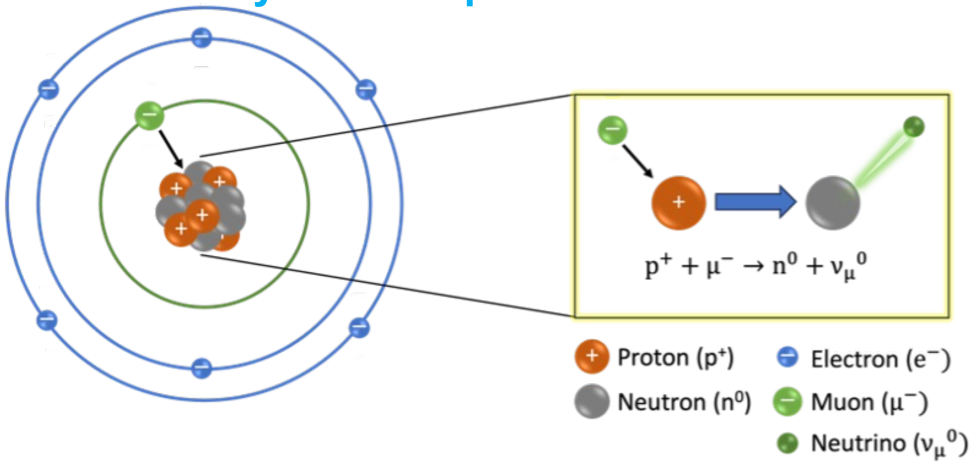
Discrepancy between experimental and theoretical β-decay rates resolved from first principles

P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

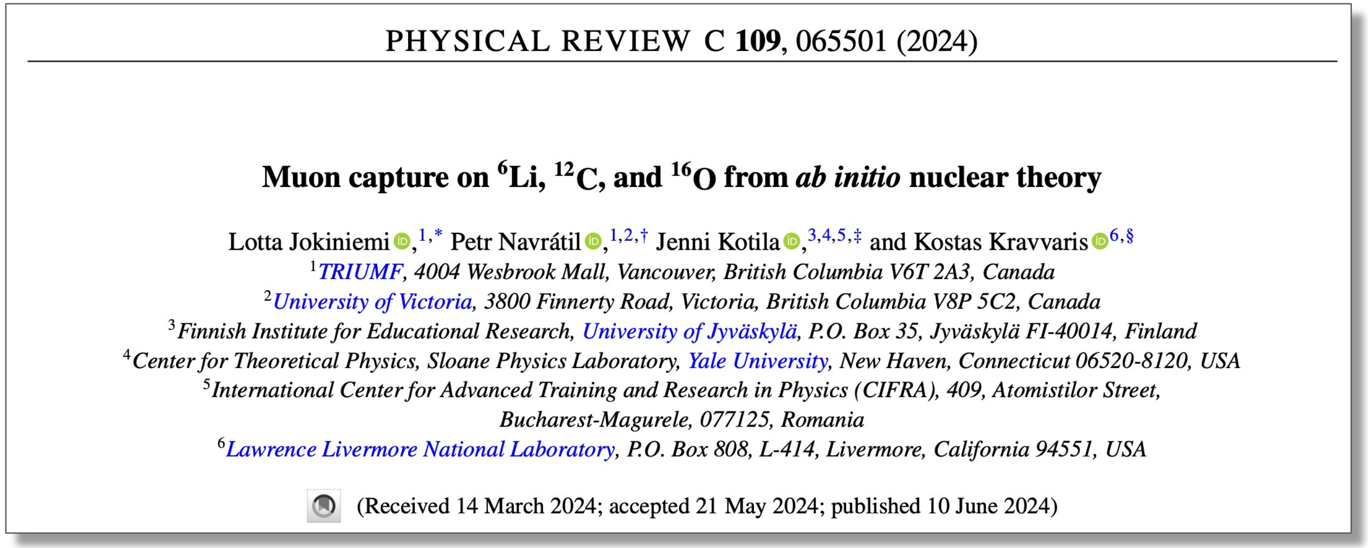
Strong nuclear correlations and two-body currents solve the beta decay quenching problem

Muon capture on ^{6}Li, ^{12}C, ^{16}N from *ab initio* nuclear theory

Ordinary muon capture on a nucleus



- ❑ Momentum exchange $q = m_\mu + E_i - E_f \approx 100$ MeV
- ❑ Involves vector, axial-vector, magnetic and pseudoscalar nuclear-weak currents
  → **Can be used as a probe of $0\nu\beta\beta$ decay**

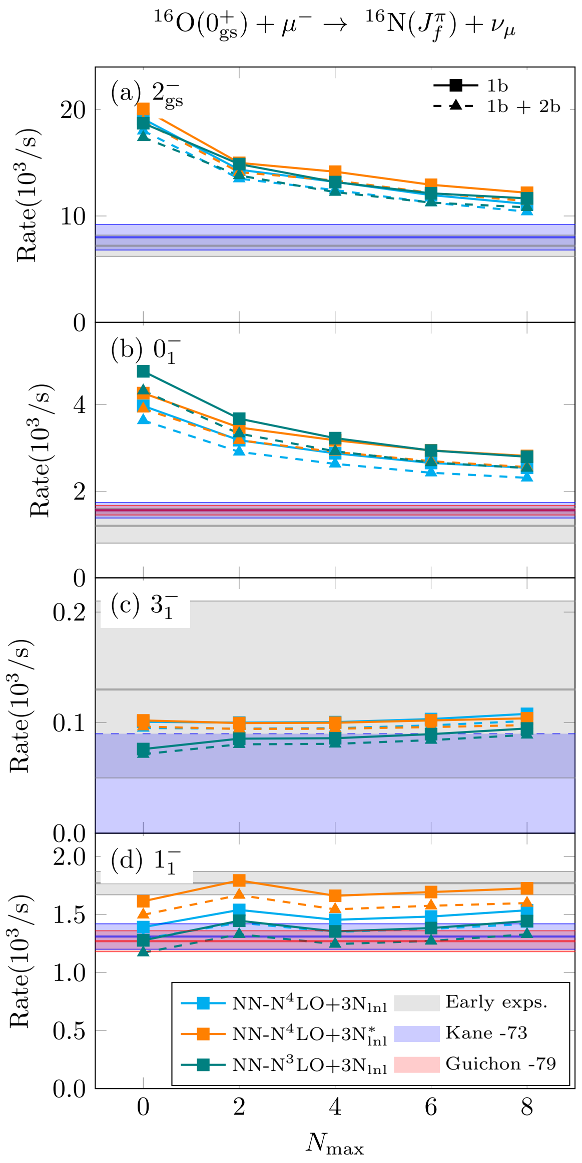


PHYSICAL REVIEW C **109**, 065501 (2024)

Muon capture on ^{6}Li, ^{12}C, and ^{16}O from *ab initio* nuclear theory

Lotta Jokiniemi,[1,*] Petr Navrátil,[1,2,†] Jenni Kotila,[3,4,5,‡] and Kostas Kravvaris[6,§]
[1]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*
[2]*University of Victoria, 3800 Finnerty Road, Victoria, British Columbia V8P 5C2, Canada*
[3]*Finnish Institute for Educational Research, University of Jyväskylä, P.O. Box 35, Jyväskylä FI-40014, Finland*
[4]*Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, Connecticut 06520-8120, USA*
[5]*International Center for Advanced Training and Research in Physics (CIFRA), 409, Atomistilor Street, Bucharest-Magurele, 077125, Romania*
[6]*Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA*

(Received 14 March 2024; accepted 21 May 2024; published 10 June 2024)



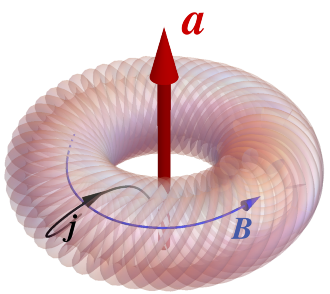
- ❑ ***Ab initio no-core*** **shell-model calculations in good agreement with experiments**

See talk by Lotta Jokiniemi on Saturday

NCSM applications to parity-violating moments:
How to calculate the sum of intermediate unnatural parity states?

$$a_s = \langle \psi_{\rm gs}\ I\ I_z{=}I | \hat{a}^{(1)}_{s,0} | \psi_{\rm gs}\ I\ I_z{=}I \rangle$$

$$|\psi_{\rm gs}\ I\rangle = |\psi_{\rm gs}\ I^{\pi}\rangle + \sum_j |\psi_j\ I^{-\pi}\rangle \frac{1}{E_{\rm gs} - E_j} \langle \psi_j\ I^{-\pi} | V_{\rm NN}^{\rm PNC} | \psi_{\rm gs}\ I^{\pi}\rangle$$



- Solving Schroedinger equation with inhomogeneous term

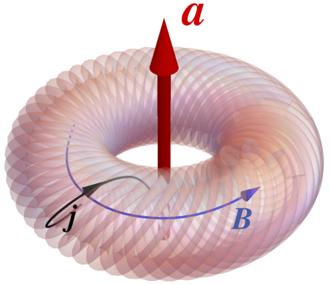
$$(E_{\rm gs} - H)|\psi_{\rm gs}\ I\rangle = V_{\rm NN}^{\rm PNC} |\psi_{\rm gs}\ I^{\pi}\rangle$$

- To invert this equation, we apply the Lanczos algorithm

NCSM applications to parity-violating moments:
How to calculate the sum of intermediate unnatural parity states?

$$a_s = \langle \psi_{\rm gs}\ I\ I_z{=}I | \hat{a}^{(1)}_{s,0} | \psi_{\rm gs}\ I\ I_z{=}I \rangle$$

$$|\psi_{\rm gs}\ I\rangle = |\psi_{\rm gs}\ I^\pi\rangle + \sum_j |\psi_j\ I^{-\pi}\rangle \frac{1}{E_{\rm gs} - E_j} \langle \psi_j\ I^{-\pi} | V^{\rm PNC}_{\rm NN} | \psi_{\rm gs}\ I^\pi\rangle$$



- Solving Schroedinger equation with inhomogeneous term

$$(E_{\rm gs} - H)|\psi_{\rm gs}\ I\rangle = V^{\rm PNC}_{\rm NN} |\psi_{\rm gs}\ I^\pi\rangle$$

- To invert this equation, we apply the Lanczos algorithm
  - Bring matrix to tri-diagonal form ($\mathbf{v}_1$, $\mathbf{v}_2$ … orthonormal, H Hermitian)

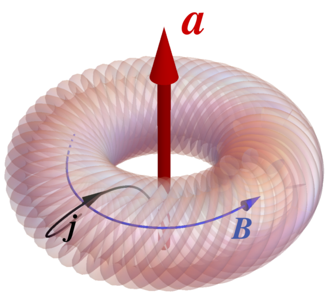
$$\begin{aligned}
H\mathbf{v}_1 &= \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2 \\
H\mathbf{v}_2 &= \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3 \\
H\mathbf{v}_3 &= \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4 \\
H\mathbf{v}_4 &= \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5
\end{aligned}$$

  - n^{th} iteration computes $2n^{th}$ moment
  - Eigenvalues converge to extreme (largest in magnitude) values
  - ~ 150-200 iterations needed for 10 eigenvalues (even for 10^9 states)

NCSM applications to parity-violating moments:
How to calculate the sum of intermediate unnatural parity states?

$$a_s = \langle \psi_{\rm gs}\ I\ I_z{=}I | \hat{a}^{(1)}_{s,0} | \psi_{\rm gs}\ I\ I_z{=}I \rangle$$

$$|\psi_{\rm gs}\ I\rangle = |\psi_{\rm gs}\ I^{\pi}\rangle + \sum_j |\psi_j\ I^{-\pi}\rangle \frac{1}{E_{\rm gs} - E_j} \langle \psi_j\ I^{-\pi} | V^{\rm PNC}_{\rm NN} | \psi_{\rm gs}\ I^{\pi}\rangle$$

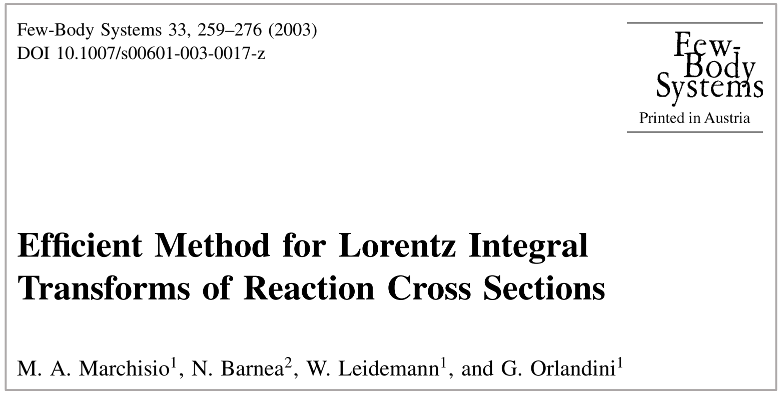


- Solving Schroedinger equation with inhomogeneous term

$$(E_{\rm gs} - H)|\psi_{\rm gs}\ I\rangle = V^{\rm PNC}_{\rm NN} |\psi_{\rm gs}\ I^{\pi}\rangle$$

- To invert this equation, we apply the Lanczos algorithm

$$|\mathbf{v}_1\rangle = V^{\rm PNC}_{\rm NN} |\psi_{\rm gs}\ I^{\pi}\rangle$$



Few-Body Systems 33, 259–276 (2003)
DOI 10.1007/s00601-003-0017-z

Few-Body Systems
Printed in Austria

Efficient Method for Lorentz Integral Transforms of Reaction Cross Sections

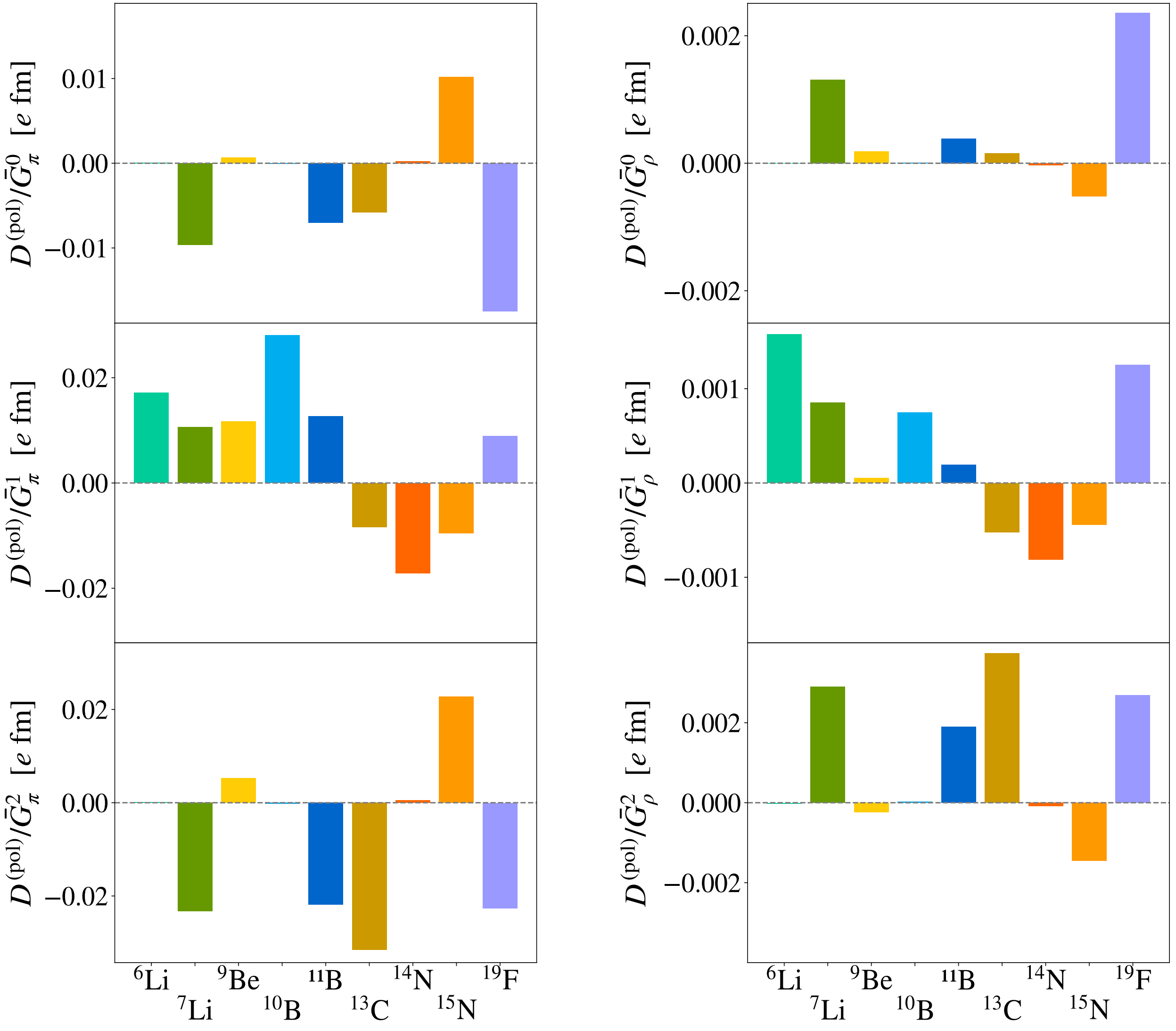
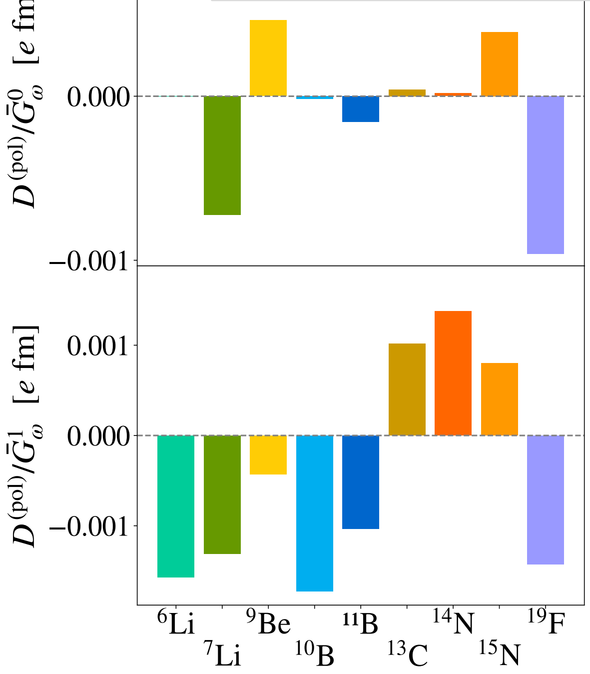
M. A. Marchisio[1], N. Barnea[2], W. Leidemann[1], and G. Orlandini[1]

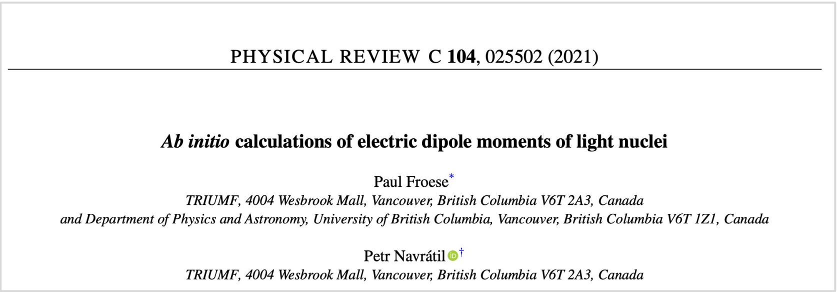
$$|\psi_{\rm gs}\ I\rangle \approx \sum_k g_k(E_0) |\mathbf{v}_k\rangle$$

$$\hat{g}_1(\omega) = \cfrac{1}{\omega - \alpha_1 - \cfrac{\beta_1^2}{\omega - \alpha_2 - \cfrac{\beta_2^2}{\omega - \alpha_3 - \beta_3^2}}} \quad \ddots$$

Lanczos continued fraction method

NCSM applications to parity-violating moments:
Anapole moments & EDMs of light stable nuclei


PHYSICAL REVIEW C **104**, 025502 (2021)

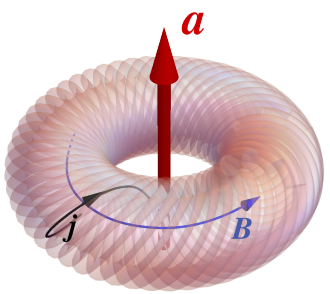
***Ab initio* calculations of electric dipole moments of light nuclei**

Paul Froese*

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada
and Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z1, Canada

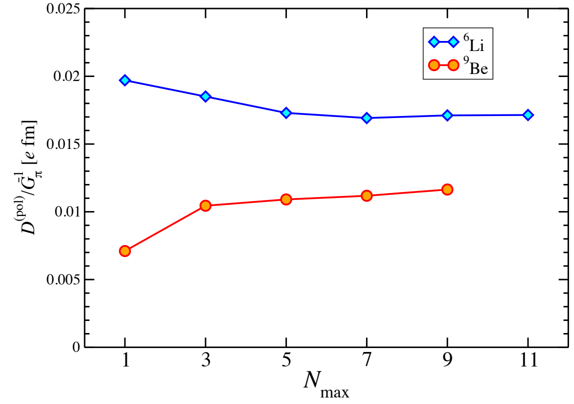
Petr Navrátil†

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada



Y. Hao, P. Navratil *et al.*, PRA **102**, 052828 (2020)

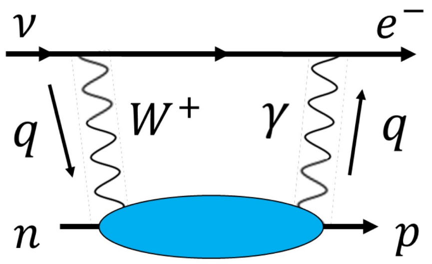
Examples of N_{max} convergence



Synergy of precision experiments and *ab initio* nuclear theory to test CKM unitarity

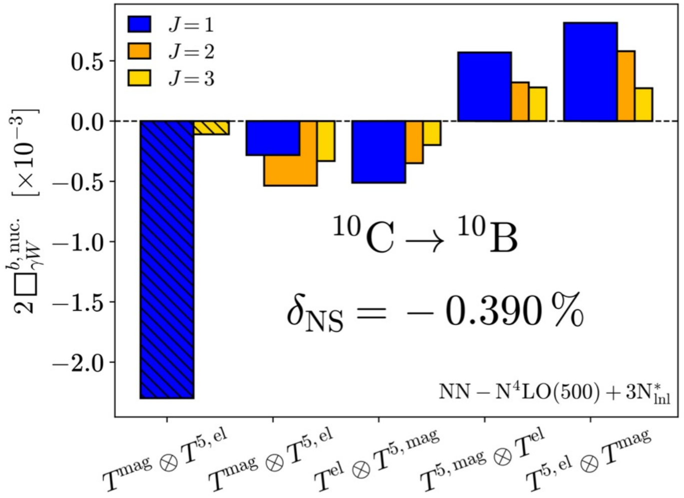
Structure corrections for the extraction of the V_{ud} matrix element from the $^{10}C \to ^{10}B$ Fermi transition

- CKM unitarity sensitive probe of BSM physics
  - V_{ud} element from super-allowed Fermi transitions



$$|V_{ud}|^2 = \frac{\hbar^7}{G_F^2 m_e^5 c^4} \frac{\pi^3 \ln(2)}{\mathcal{F}t} \qquad \mathcal{F}t = \frac{K}{G_V^2 |M_{F0}|^2 (1+\Delta_R^V)}$$

$$\mathcal{F}t(1+\Delta_R^V) = ft(1+\delta_R')(1-\delta_C+\delta_{NS})$$



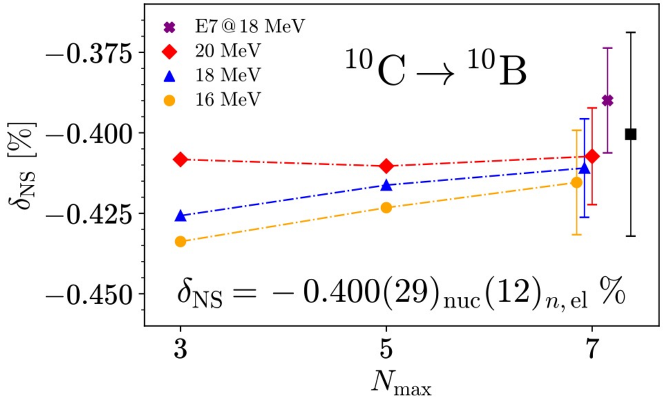
- δ_{NS} parametrizes correction to free γW box
- *Ab initio* no-core shell model (NCSM)
  - A very good convergence – consistent with what used in latest evaluation with a substantially reduced theoretical uncertainties

$$\delta_{NS} = 2[\Box_{\gamma W}^{VA,\text{nuc.}} - \Box_{\gamma W}^{VA,\text{free n}}]$$

An *ab initio* strategy for taming the nuclear-structure dependence of V_{ud} extractions: the $^{10}C \to ^{10}B$ superallowed transition

arXiv: 2405.19281

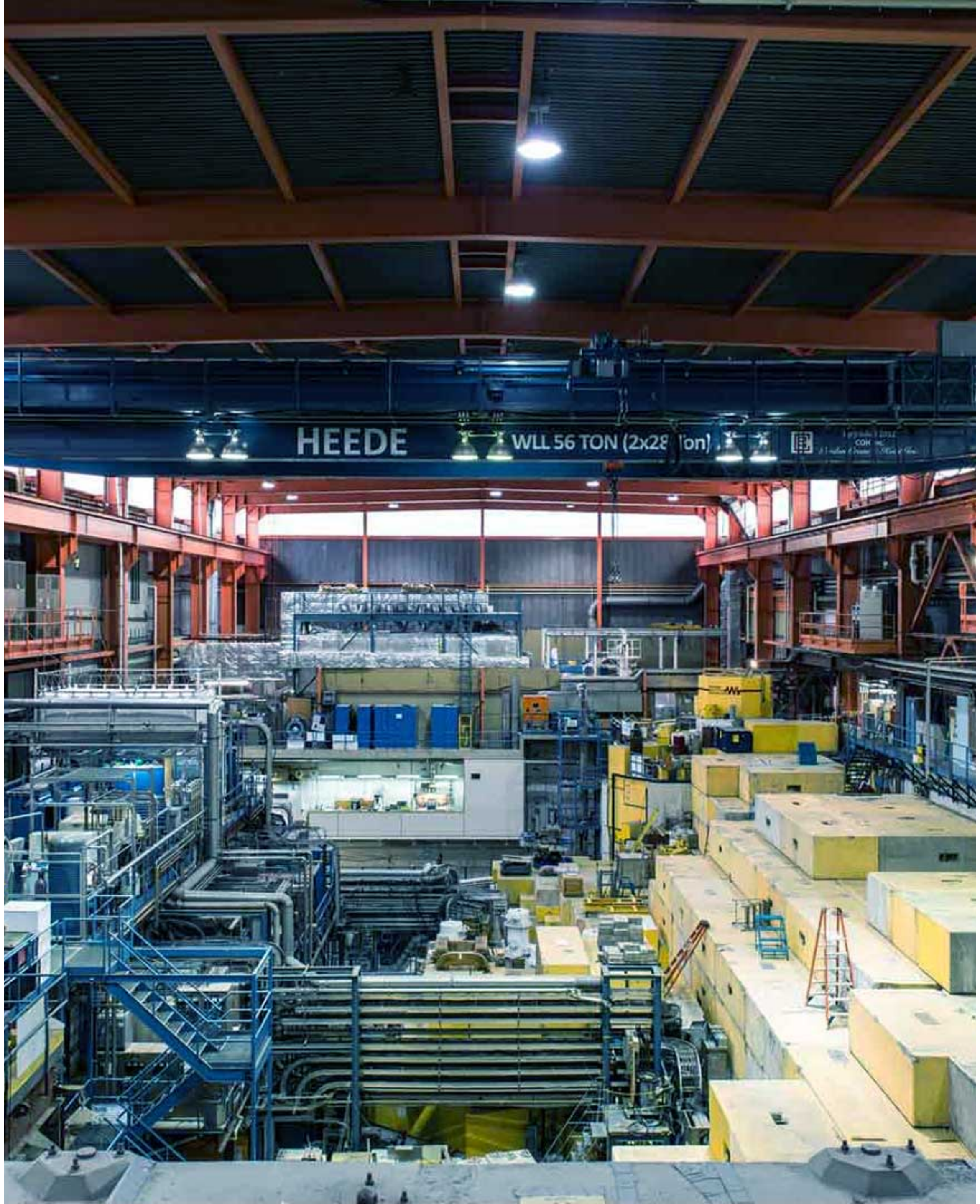
Michael Gennari[1,2], Mehdi Drissi[1], Mikhail Gorchtein[3,4], Petr Navrátil[1,2], and Chien-Yeah Seng[5,6]



NCSM applicable also to $^{14}O \to ^{14}N$ and possibly $^{18}Ne \to ^{18}F$, $^{22}Mg \to ^{22}Na$

TRIUMF

No-Core Shell Model with Continuum (NCSMC) - Unified description of bound and unbound states



Discovery, accelerated

Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

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

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

Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

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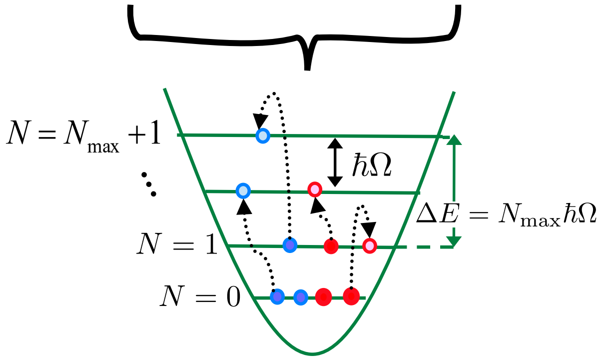

Static solutions for aggregate system, describe all nucleons close together

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

Ab Initio Calculations of Structure, Scattering, Reactions
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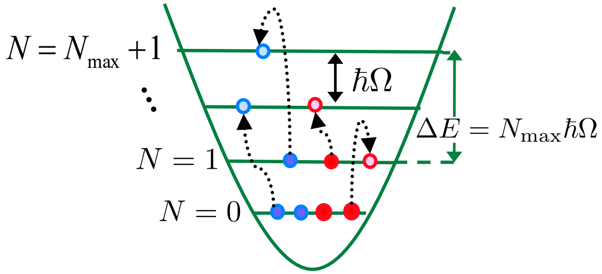
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| {}_{(A-a)} \overset{\vec{r}}{\longleftarrow} (a), \nu \right\rangle$$



Continuous microscopic cluster states, describe long-range projectile-target

Static solutions for aggregate system, describe all nucleons close together

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

See also talk by Kostas Kravvaris later today

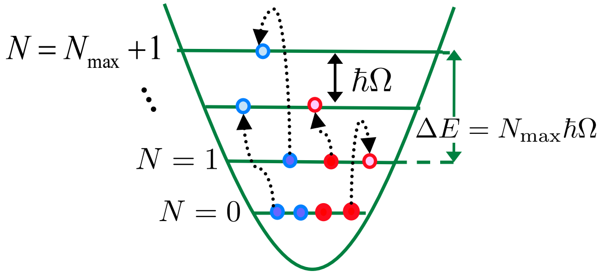
Ab Initio Calculations of Structure, Scattering, Reactions

Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

Unknowns

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



Continuous microscopic cluster states, describe long-range projectile-target

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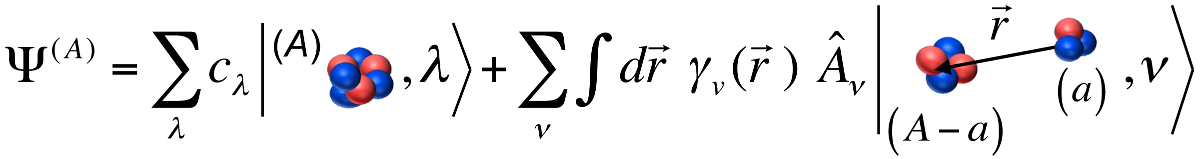
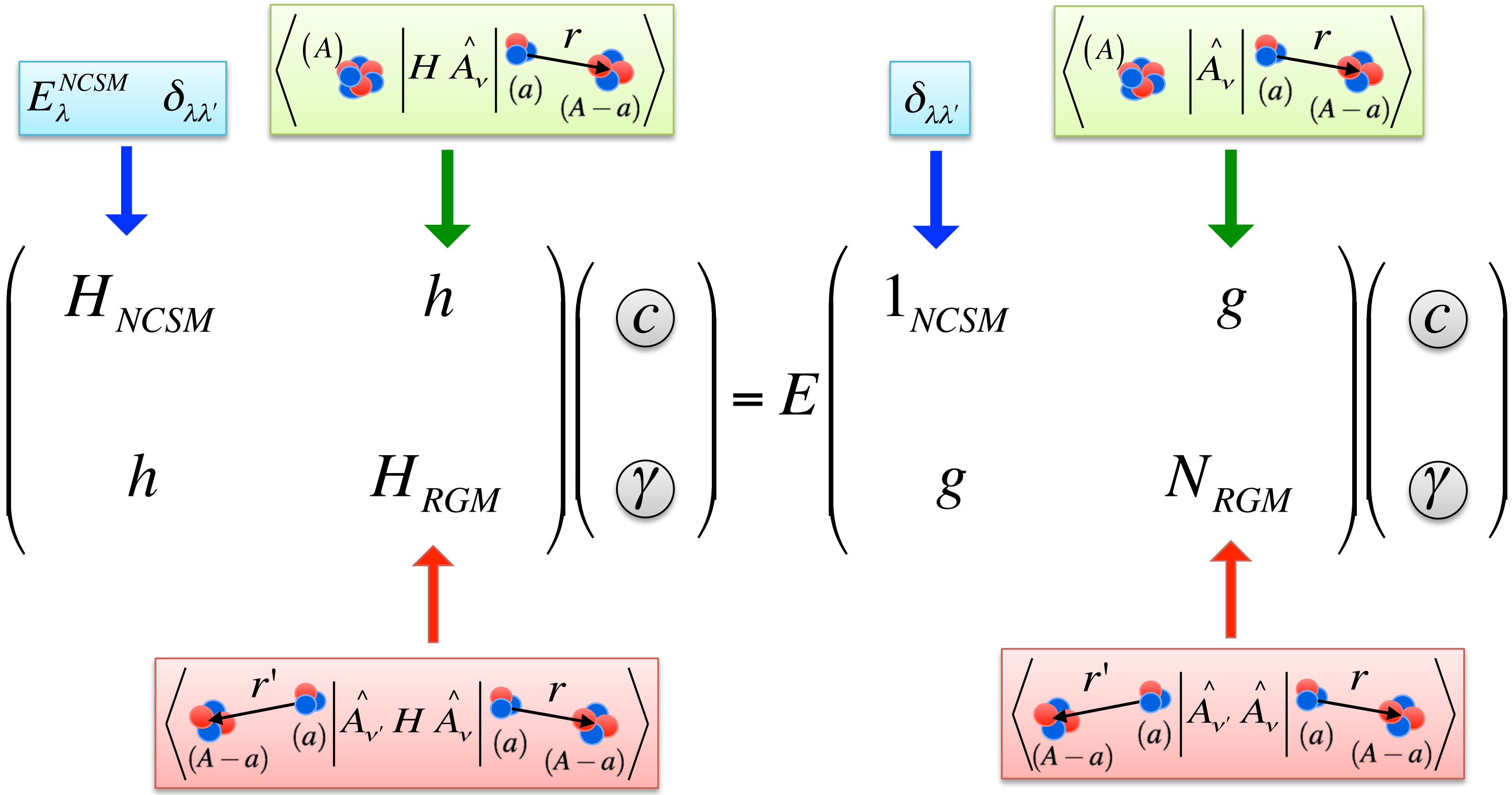
S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Coupled NCSMC equations

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





IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. **91** (2016) 053002 (38pp) doi:10.1088/0031-8949/91/5/053002

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

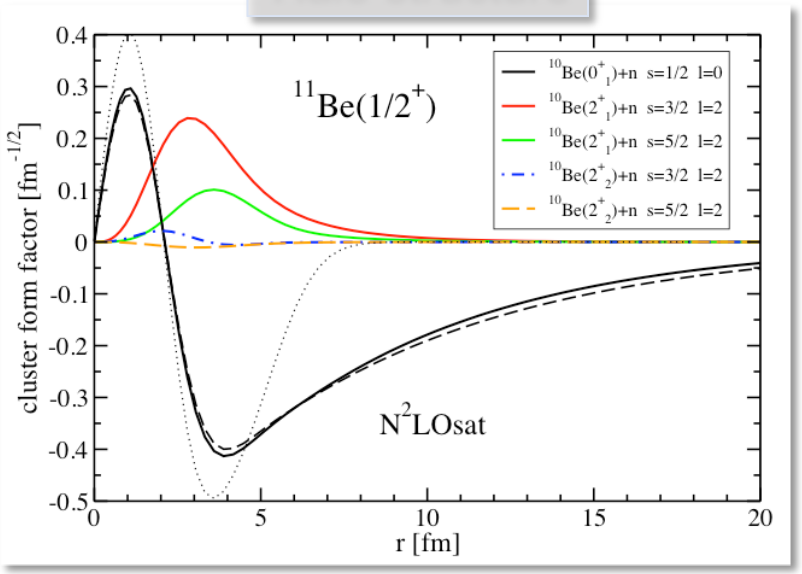
Studies of exotic nuclei – continuum effects

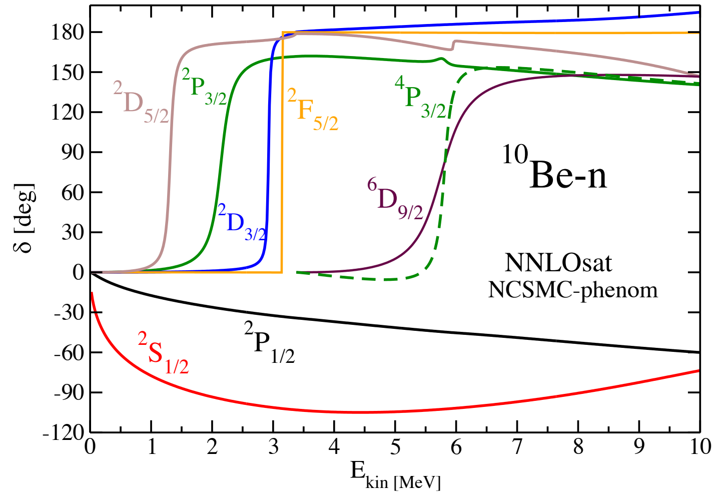
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} , \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r})\ \hat{A}_{\nu} \left| {}_{(A-a)} \vec{r}\ {}_{(a)} , \nu \right\rangle$$

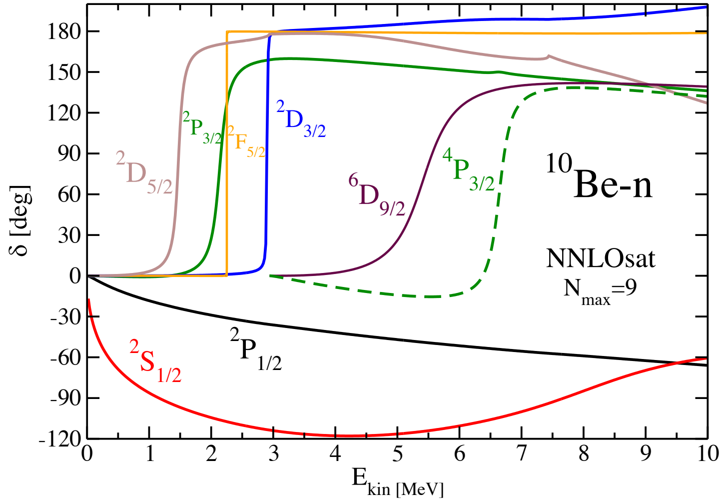
Photo-disassociation of ^{11}Be

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

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

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

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]

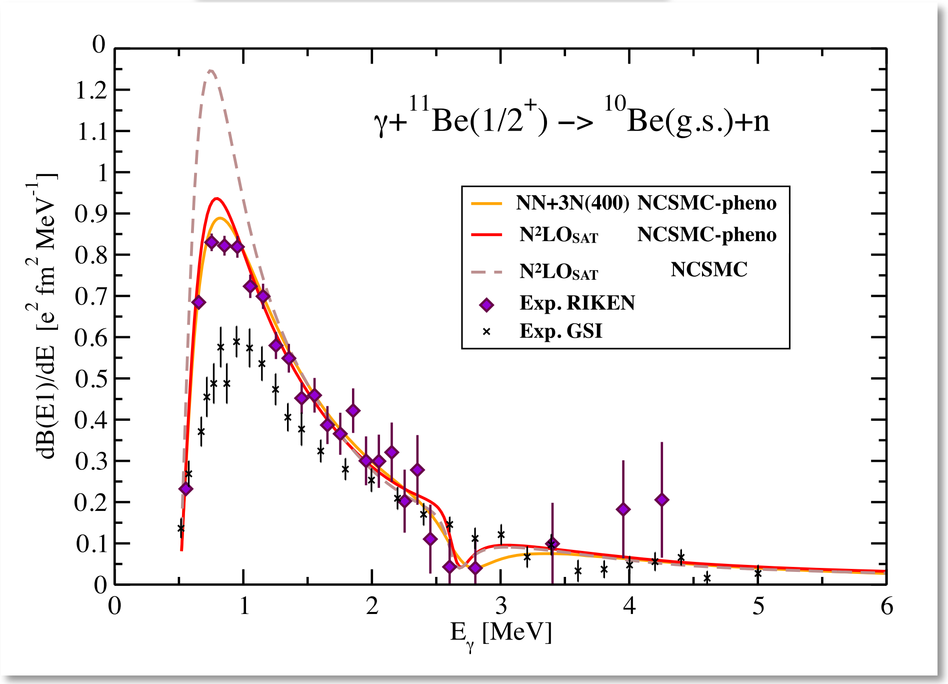
Studies of exotic nuclei – continuum effects

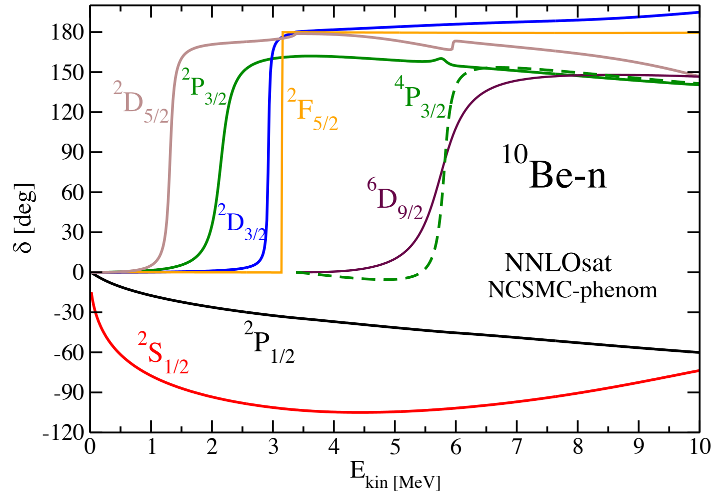
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r})\; \hat{A}_{\nu} \left| {}_{(A-a)} \overset{\vec{r}}{\longrightarrow} {}_{(a)}, \nu \right\rangle$$

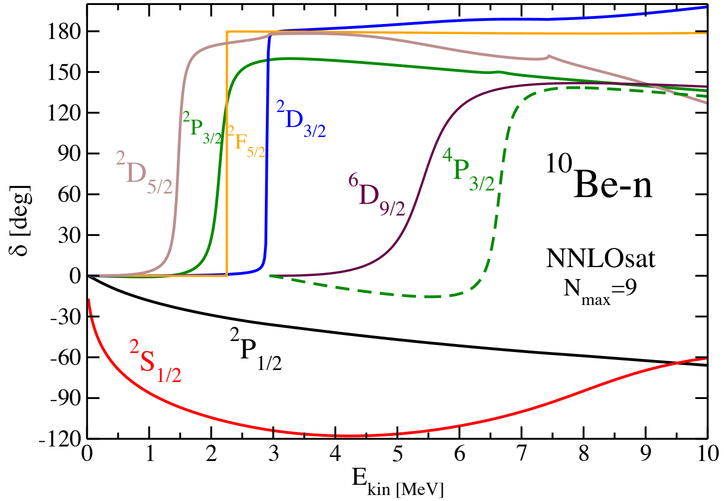
Photo-disassociation of ^{11}Be

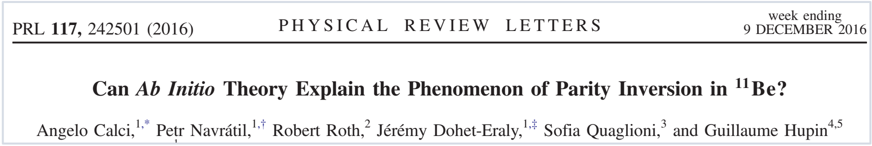
Bound to bound	NCSM	NCSMC-phenom	Expt.
B(E1; $1/2^{+} \rightarrow 1/2^{-}$) [$e^2$ fm^2]	0.0005	0.117	0.102(2)

Bound to continuum








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]

Radiative Capture Reaction: $^4He(d,\gamma)^6Li$

Responsible for ^6Li production in BBN – 10^3 discrepancy between theory/observation

Deficiency in observation, theory, or new physics?

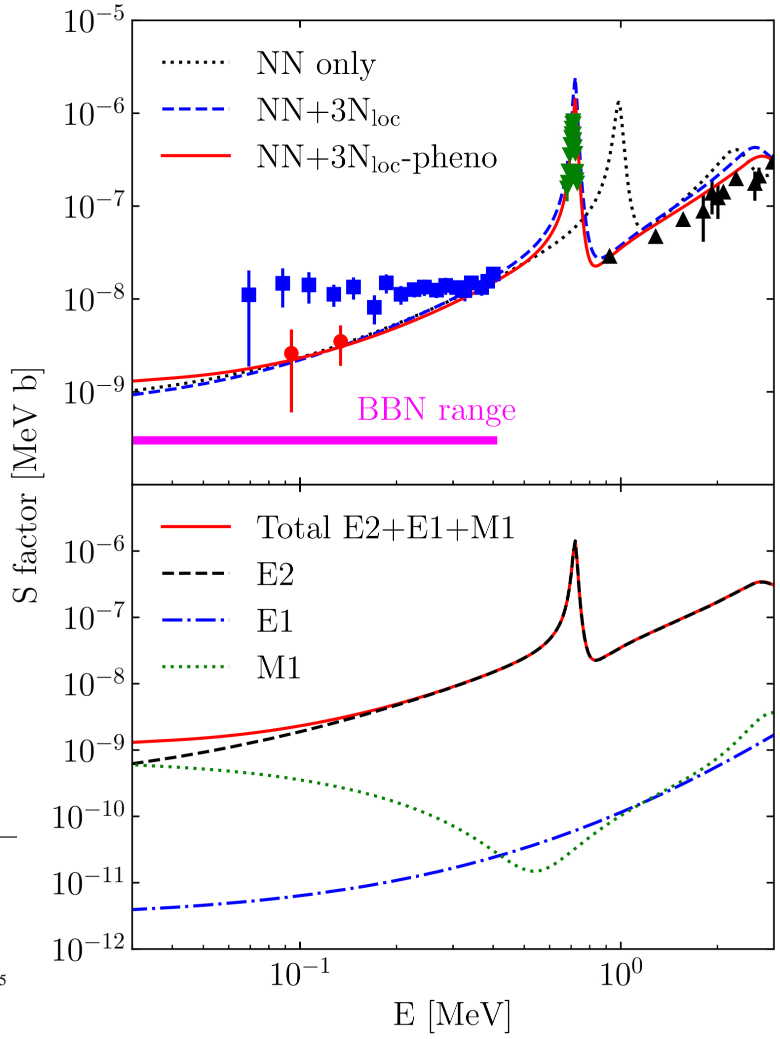
NCSMC calculation w/ chiral forces

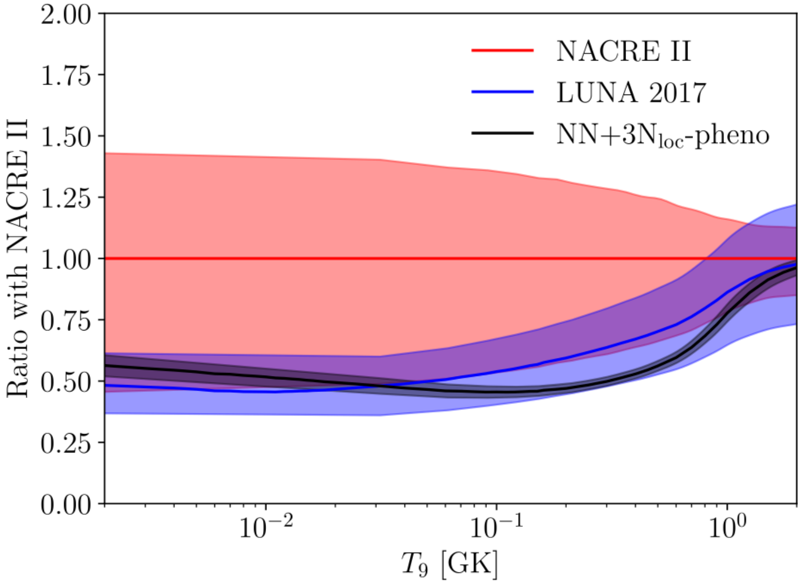
Radiative capture S-factor

- Dominated by *E2*
- *M1* significant at low energy
- *E1* negligible (isospin supressed)

Thermonuclear reaction rate

- Smaller than NACRE II evaluation
- Agrees w/ LUNA; reduced uncertainty





PHYSICAL REVIEW LETTERS **129,** 042503 (2022)

***Ab Initio* Prediction of the $^4He(d,\gamma)^6Li$ Big Bang Radiative Capture**

C. Hebborn,[1,2,*] G. Hupin,[3] K. Kravvaris,[2] S. Quaglioni,[2] P. Navrátil,[4] and P. Gysbers[4,5]

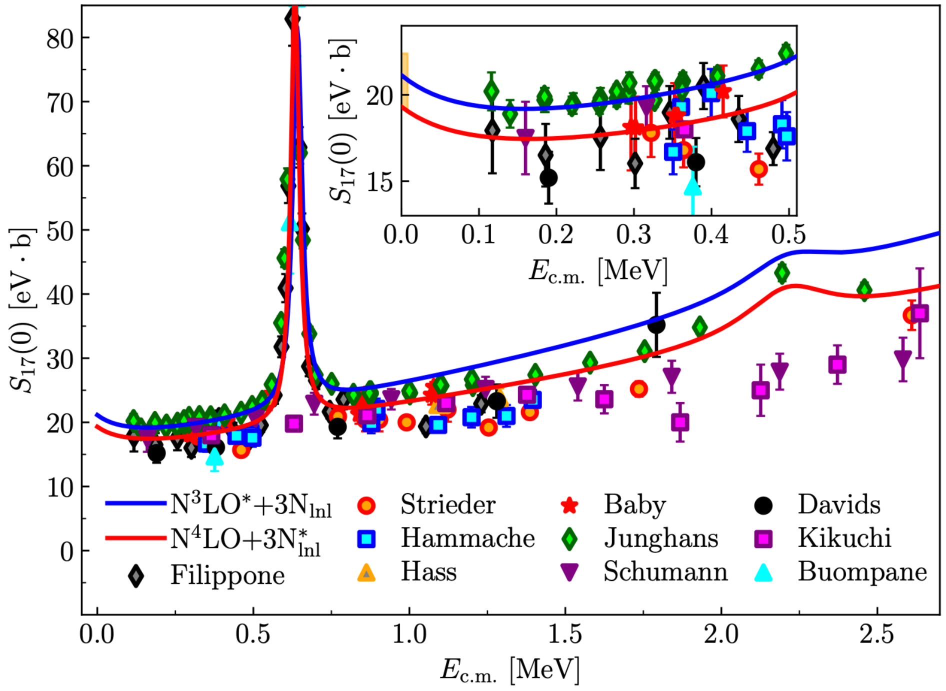
Radiative capture of protons on ^{7}Be

- Solar pp chain reaction, solar ^{8}B neutrinos
- NCSMC calculations with a set of chiral NN+3N interactions as input
  - Radiative capture S-factor
    - Dominated by *E1* non-resonant
    - *M1/E2* significant at 1^+ and 3^+ resonances
  - Correlations between results obtained by different chiral interactions and experimental data → evaluation of the S-factor at *E*=0 energy relevant for the solar physics

Recommended value $S_{17}(0)$ ~ 19.8(3) eV b

Latest evaluation in *Rev. Mod. Phys.* **83,**195–245 (2011):
$S_{17}(0)$ = 20.8 ± 0.7(expt) ± 1.4(theory) eV b

^{7}Be(p,γ)^{8}B



Physics Letters B 845 (2023) 138156

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/physletb

Ab initio informed evaluation of the radiative capture of protons on ^{7}Be

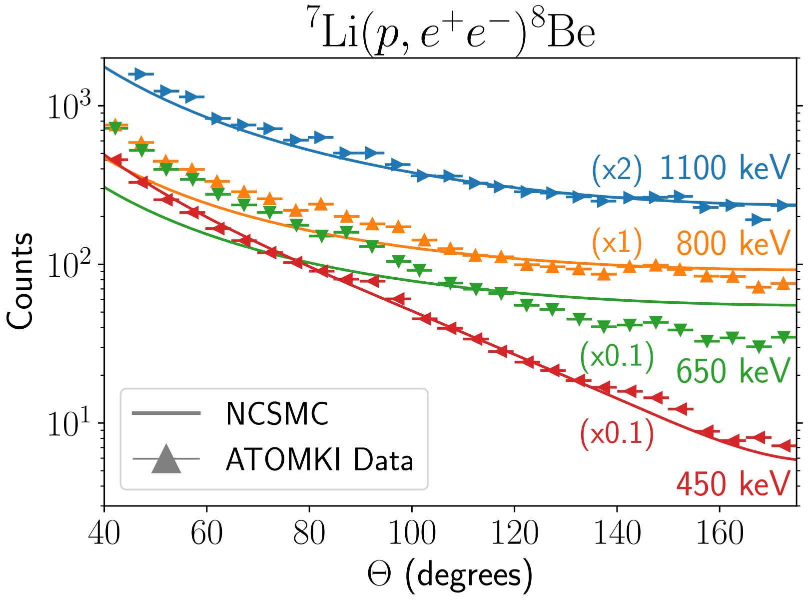
K. Kravvaris [a,*], P. Navrátil [b], S. Quaglioni [a], C. Hebborn [c,a], G. Hupin [d]

See talk by Peter Gysbers on Sunday

Recently developed NCSMC capability – charge-exchange reaction calculations

- The first published application - ^{7}Li+p scattering and radiative capture
  - Wave function ansatz

$$\Psi^{(8)}_{\text{NCSMC}} = \sum_{\lambda} c_\lambda \left|{}^8\text{Be}, \lambda\right\rangle + \sum_{\nu} \int dr \gamma_\nu(r) \hat{A}_\nu \left|{}^7\text{Li} + p, \nu\right\rangle + \sum_{\mu} \int dr \gamma_\mu(r) \hat{A}_\mu \left|{}^7\text{Be} + n, \mu\right\rangle$$

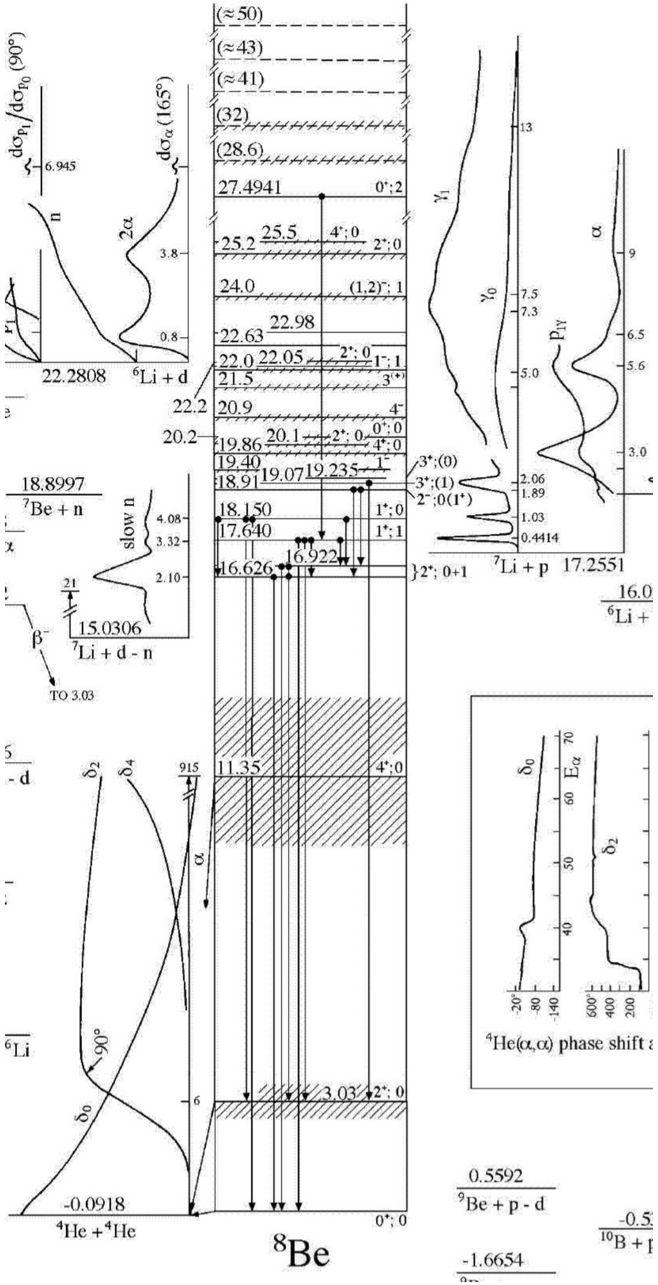


PHYSICAL REVIEW C **110**, 015503 (2024)

Editors' Suggestion

***Ab initio* investigation of the ^{7}Li$(p, e^+e^-)^8$Be process and the X17 boson**

P. Gysbers,[1,2,3] P. Navrátil,[1,4] K. Kravvaris,[5] G. Hupin,[6] and S. Quaglioni[5]



Conclusions

- *Ab initio* nuclear theory
  - Makes connections between the low-energy QCD and many-nucleon systems

- No-core shell model is an *ab initio* extension of the original nuclear shell model
  - Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries

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Thank you!
Merci!

Thanks to all my collaborators over the years!

Discovery, accelerated