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Ab initio nuclear reaction theory: Applications to nuclear astrophysics and the X17 boson claim

QNP2022 - The 9th International Conference on Quarks and Nuclear Physics

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2022-09-04

First principles or ab initio nuclear theory



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



Ab Initio Calculations of Structure, Scattering, Reactions Unified approach to bound & continuum states

No-Core Shell Model with Continuum (NCSMC)

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

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

$$N = N_{\max} + 1 \stackrel{\vec{h}\Omega}{\longrightarrow}_{N=1} \Delta E = N_{\max} \hbar \Omega$$

$$N = 0$$

Static solutions for aggregate system, describe all nucleons close together

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

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No-Core Shell Model with Continuum (NCSMC)



Static solutions for aggregate system, describe all nucleons close together

Coupled NCSMC equations

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

$$E_{\lambda}^{NCSM} \delta_{\lambda\lambda'} \qquad \begin{pmatrix} (A) \bigotimes |H \hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ H_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle (A) \bigotimes |\hat{A}_{\nu}|_{(a)}^{\vec{r}} (a) \rangle \\ \downarrow \\ I_{NCSM} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \delta_{\lambda\lambda'} & \delta_{\lambda\lambda'} & \delta_{\lambda\lambda'} & \delta_{\lambda\lambda'} \\ \downarrow \\ I_{NCSM} & I_{NCSM} \end{pmatrix}$$

Physica Scripta doi:10.1088/0031-8949/91/5/053002 Royal Swedish Academy of Scie 053002 (38pp)

8

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d ab initio approaches to nuclear structure and reactions

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4}, Carolina Romero-Redondo² and Angelo Calci¹

Input for NCSMC calculations: Nuclear forces from chiral Effective Field Theory

- Approach taking advantage of the separation of scales
 - 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_x)
 - Hierarchy
 - Consistency
 - Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD



 Λ_{χ} ~1 GeV : Chiral symmetry breaking scale

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,∥}

Input for NCSMC calculations: Nuclear 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, ³H and ⁴He binding energy, ³H half life
 - Light nuclei NCSM
 - Medium mass nuclei Self-Consistent Green's Function method

NN N³LO (Entem-Machleidt 2003) 3N N²LO w local/non-local regulator



PHYSICAL	REVIEW	C 101,	, 014318	(2020)
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 - Light nuclei NCSM
 - Heavy nuclei HF-MBPT(3)





β-delayed proton emission in ¹¹Be

12





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Physics Letters B

Physics Letters B 732 (2014) 305-308

¹¹Be(β p), a quasi-free neutron decay?

K. Riisager^{a,*}, O. Forstner^{b,c}, M.J.G. Borge^{d,e}, J.A. Briz^e, M. Carmona-Gallardo^e, L.M. Fraile^f, H.O.U. Fynbo^a, T. Giles^g, A. Gottberg^{e,g}, A. Heinz^h, J.G. Johansen^{a,1}, B. Jonson^h, J. Kurcewicz^d, M.V. Lund^a, T. Nilsson^h, G. Nyman^h, E. Rapisarda^d, P. Steier^b, O. Tengblad^e, R. Thies^h, S.R. Winkler^b

- Indirectly observed ${}^{11}\text{Be}(\beta p){}^{10}\text{Be}$
- Measured an extremely high branching ratio $b_p = 8.3 \pm 0.9 \times 10^{-6}$
 - Orders of magnitude larger than theoretical predictions (e.g. 3.0×10^{-8})
- Two proposed explanations:

D. Baye and E.M. Tursunov, PLB 696, 4, 464-467 (2011)

- The neutron decays to an unobserved $p+^{10}Be$ resonance in ¹¹B
- 2 There are unobserved dark decay modes

β-delayed proton emission in ¹¹Be

PHYSICAL REVIEW LETTERS 123, 082501 (2019)

Editors' Suggestion

Direct Observation of Proton Emission in ¹¹Be

Y. Ayyad,^{1,2,*} B. Olaizola,³ W. Mittig,^{2,4} G. Potel,¹ V. Zelevinsky,^{1,2,4} M. Horoi,⁵ S. Beceiro-Novo,⁴ M. Alcorta,³
C. Andreoiu,⁶ T. Ahn,⁷ M. Anholm,^{3,8} L. Atar,⁹ A. Babu,³ D. Bazin,^{2,4} N. Bernier,^{3,10} S. S. Bhattacharjee,³ M. Bowry,³
R. Caballero-Folch,³ M. Cortesi,² C. Dalitz,¹¹ E. Dunling,^{3,12} A. B. Garnsworthy,³ M. Holl,^{3,13} B. Kootte,^{3,8}
K. G. Leach,¹⁴ J. S. Randhawa,² Y. Saito,^{3,10} C. Santamaria,¹⁵ P. Šiurytė,^{3,16} C. E. Svensson,⁹
R. Umashankar,³ N. Watwood,² and D. Yates^{3,10}

- Directly observed the protons from ${}^{11}\text{Be}(\beta p){}^{10}\text{Be}$
- Measured consistent branching ratio $b_p = 1.3(3) \times 10^{-5}$
 - Still orders of magnitude larger than theoretical predictions
- Predict the proton resonance at 11.425(20) MeV from the proton energy distribution
 - Predicted to be either $\frac{1}{2}^+$ or $\frac{3}{2}^+$
 - Corresponds to excitation energy of 197 keV

NCSMC extended to describe exotic ¹¹Be β p emission, supports large branching ratio due to narrow $\frac{1}{2}$ resonance

¹¹Be \rightarrow (¹⁰Be+p) + β^- + $\bar{\nu}_e$ GT transition



NCSMC extended to describe exotic ¹¹Be β p emission, supports large branching ratio due to narrow $\frac{1}{2}$ resonance



NCSMC extended to describe exotic ¹¹Be β p emission, supports large branching ratio due to narrow ¹/₂+ resonance



Radiative capture of deuterons on ⁴**He**

- Reaction ${}^{4}\text{He}(d,\gamma){}^{6}\text{Li}$ responsible for ${}^{6}\text{Li}$ production in BBN
- Three orders of magnitude discrepancy between BBN predictions and observations
 - Problem with astronomical observations?
 - Problem with our understanding of the reaction rate?
 - New physics?



Radiative capture of deuterons on ⁴**He**

NCSMC calculations with chiral NN+3N interaction



Structure of ⁶Li

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

C. Hebborn⁽⁰⁾,^{1,2,*} G. Hupin⁽⁰⁾,³ K. Kravvaris⁽⁰⁾,² S. Quaglioni⁽⁰⁾,² P. Navrátil⁽⁰⁾,⁴ and P. Gysbers⁽⁰⁾,⁵

Ground state properties: Energy Asymptotic normalization constants Magnetic moment

	NN-only	$3 \mathrm{N}_\mathrm{loc}$	$3N_{loc}$ -pheno	Exp. or Eval.
$E_{\rm g.s.}$	-1.848	-1.778	-1.474	-1.4743
\mathcal{C}_0	2.95	2.89	2.62(4)	2.28(7) 2.29(12)
\mathcal{C}_2	-0.0369	-0.0642	-0.0554(305)	-0.077(18)
$\mathcal{C}_2/\mathcal{C}_0$	-0.013	-0.022	-0.021(11)	-0.025(6)(10)
μ	0.85	0.84	0.84(1)	0.8220473(6)

⁴He+*d* threshold

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C. Hebborn⁰,^{1,2,*} G. Hupin⁰,³ K. Kravvaris⁰,² S. Quaglioni⁰,² P. Navrátil⁰,⁴ and P. Gysbers^{04,5}

NCSMC calculations with chiral NN+3N interaction

Radiative capture of deuterons on ⁴He



Structure of ⁶Li

Elastic scattering ${}^{4}\text{He}(d,d){}^{4}\text{He}$ cross section at the deuteron back scattered angle 164°



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

C. Hebborn^(0,1,2,*) G. Hupin^(0,3) K. Kravvaris^(0,2) S. Quaglioni^(0,2) P. Navrátil^(0,4) and P. Gysbers^(0,4,5)

Radiative capture of deuterons on ⁴**He**

- NCSMC calculations with chiral NN+3N interaction
 - Capture S-factor

Dominated by E2 M1 significant at low energy E1 negligible – isospin supressed (T=0 \rightarrow T=0)





Low energy S-factor consistent with LUNA data, below the ⁶Li Coulomb breakup data

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

21

C. Hebborn⁰,^{1,2,*} G. Hupin⁰,³ K. Kravvaris⁰,² S. Quaglioni⁰,² P. Navrátil⁰,⁴ and P. Gysbers^{04,5}

Radiative capture of deuterons on ⁴He

- NCSMC calculations with chiral NN+3N interaction
 - Thermonuclear reaction rate



Thermonuclear reaction rate smaller than NACRE II evaluation, agreement with LUNA result with less uncertainty

Ab initio prediction for the radiative capture of protons on ⁷Be

K. Kravvaris,¹ P. Navrátil,² S. Quaglioni,¹ C. Hebborn,^{3,1} and G. Hupin⁴

arXiv: 2202.11759

Radiative capture of protons on 7Be

- Solar pp chain reaction, solar ⁸B neutrinos
- NCSMC calculations with a set of chiral NN+3N interactions as input
- Example of ⁸B structure results



Radiative capture of protons on 7Be

NCSMC S-factor results



E1 non-resonant, M1/E2 at 1⁺ and 3⁺ resonances

	$C_{p_{1/2}}$	$C_{p_{3/2}}$	a_1	a_2	$S_{17}(0)$
N^2LO+3N_{lnl}	0.384	0.691	4.4(1)	-0.5(1)	23.9
$N^{3}LO + 3N_{1nl}$	0.390	0.678	1.3(1)	-4.7(1)	23.5
$N^4LO + 3N_{\rm lnl}$	0.354	0.669	1.6(1)	-4.4(1)	22.0
$N^4LO+3N^*_{lnl}$	0.343	0.621	1.3(1)	-5.0(1)	19.3
$N^3LO^*{+}3N_{\rm lnl}$	0.334	0.663	0.1(1)	-7.7(1)	21.1
$N^{3}LO^{*}+3N_{loc}$	0.308	0.584	2.5(1)	-3.6(2)	16.8
Ref. [41]	0.315(9)	0.66(2)	$17.34^{+1.11}_{-1.33}$	$-3.18^{+0.55}_{-0.50}$	



Ab initio prediction for the radiative capture of protons on ⁷Be K. Kravvaris,¹ P. Navrátil,² S. Quaglioni,¹ C. Hebborn,^{3,1} and G. Hupin⁴ arXiv: 2202.11759

Radiative capture of protons on 7Be

NCSMC S-factor results



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Radiative capture of protons on 7Be

NCSMC S-factor results



Recommended value $S_{17}(0) \sim 19.8(3) \text{ eV b}$

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

	$C_{p_{1/2}}$	$C_{p_{3/2}}$	a_1	a_2	$S_{17}(0)$
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X17 Anomaly



Feng PRD 95, 035017 (2017)

"An anomaly in the internal pair creation on the M1 transition depopulating the 18.15 MeV isoscalar 1^+ state on ${}^8\text{Be}$ was observed. This could be explained by the creation and subsequent decay of a new boson .. mass 17.01(16) MeV"



Fig. from PLB 813, 136061 (2021)

NCSMC calculations of ⁸Be structure and ⁷Li+p scattering and capture

Wave function ansatz

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

- 3/2⁻, 1/2⁻, 7/2⁻, 5/2⁻, 5/2⁻ ⁷Li and ⁷Be states in cluster basis
- 15 positive and 15 negative parity states in ⁸Be composite state basis



In collaboration with UBC/TRIUMF PhD student Peter Gysbers

TUNL Nuclear Data Evaluation Project

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⁸Be structure

Calculated ⁸Be bound states w.r.t. ⁷Li + p threshold ($N_{max} = 8/9$)

State	Energy [MeV]		Excitation Energy [MeV]	
	NCSMC	Expt.	NCSMC	Expt.
0^+	-16.13	-17.25	0.00	0.00
2^+	-12.72	-14.23	3.41	3.03
4^+	-4.31	-5.91	11.82	11.35
2^+	-0.10	-0.63	16.03	16.63
2^+	+0.31	-0.33	16.44	16.92

Matches experiment well, except the 3rd 2^+ is slightly above the $^7{\rm Li} + p$ threshold.





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⁸Be structure – calculated positive-parity eigenphase shifts



- Motivated by ATOMKI experiments (Firak, Krasznahorkay et al., EPJ Web of Conferences 232, 04005 (2020))
- No-core shell model with continuum (NCSMC) with wave function ansatz

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



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Internal electron-positron pair conversion correlation



- Motivated by ATOMKI experiments (Firak, Krasznahorkay et al., EPJ Web of Conferences 232, 04005 (2020))
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Data: Zahnow *et al.* Z.Phys.A **351** 229-236 (1995)



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- No-core shell model with continuum (NCSMC) with wave function ansatz

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



Data: Zahnow *et al.* Z.Phys.A **351** 229-236 (1995) Latest developments (arXiv: 2205.07744): Anomaly in E1 direct capture – X17 a vector boson



... more calculations to do

Conclusions

Ab initio nuclear theory

- Makes connections between the low-energy QCD and many-nucleon systems
- Applicable to nuclear structure, reactions including those relevant for astrophysics, electroweak processes, tests of fundamental symmetries
- Very recently reach extended to heavy nuclei
- Applications of *ab initio* NCSMC to
 - ¹¹Be β decay with the proton emission
 - Radiative capture of protons on ⁷Be and deuteron capture on ⁴He
 - Proton capture on ⁷Li internal pair conversion and the X17 boson claim

In synergy with experiments, ab initio nuclear theory is the right approach to understand low-energy properties of atomic nuclei

∂TRIUMF

Thank you! Merci!



Discovery, accelerated