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Halo and unbound light nuclei from *ab initio* theory

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Discovery, accelerated

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- Introduction to ab initio No-Core Shell Model with Continuum (NCSMC)
- Polarized ³H(d,n)⁴He fusion
- ¹¹Be parity inversion in low-lying states, photo-dissociation
- Structure of the halo sd-shell nucleus ¹⁵C & unbound mirror ¹⁵F

First principles or ab initio nuclear theory



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



Ab initio

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- ♦ Degrees of freedom: Nucleons
- ♦ All nucleons are active
- ♦ Exact Pauli principle
- Realistic inter-nucleon interactions
 Accurate description of NN (and 3N) data

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♦ Controllable approximations

Conceptually simplest *ab initio* method: No-Core Shell Model (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 – ⁴He, ¹⁶O, ⁴⁰Ca)
 - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances

(A)
$$\Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_{1}, \vec{\eta}_{2}, ..., \vec{\eta}_{A-1})$$

(A)
$$\Psi_{SD}^{A} = \sum_{N=0}^{N_{max}} \sum_{j} c_{Nj}^{SD} \Phi_{SDNj}^{HO}(\vec{r}_{1}, \vec{r}_{2}, ..., \vec{r}_{A}) = \Psi^{A} \varphi_{000}(\vec{R}_{CM})$$





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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...

NCSM

$$\begin{split} & \Psi^{A} = \sum_{N=0}^{N_{\text{max}}} \sum_{i} c_{Ni} \Phi^{A}_{Ni} \\ |\Psi^{J^{\pi}T}_{A}\rangle = \sum_{\nu} \int d\vec{r} \chi_{\nu}(\vec{r}) \hat{A} \Phi^{J^{\pi}T(A-a,a)}_{\nu \vec{r}} \\ & \mathcal{H}\chi = E \mathcal{N}\chi \\ & \bar{\chi} = \mathcal{N}^{+\frac{1}{2}}\chi \qquad (\mathcal{N}^{-\frac{1}{2}} \mathcal{H} \mathcal{N}^{-\frac{1}{2}}) \bar{\chi} = E \bar{\chi} \end{split}$$





Extending no-core shell model beyond bound states

Include more many nucleon correlations...

NCSM

$$\begin{split}
\Psi^{A} &= \sum_{\nu=0}^{N_{max}} \sum_{i} c_{Ni} \Phi_{Ni}^{A} \\
&|\Psi_{A}^{J^{\pi}T}\rangle = \sum_{\nu} \int d\vec{r} \chi_{\nu}(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^{\pi}T(A-a,a)} \\
&\stackrel{H}{\longrightarrow} \chi^{a} = \sum_{\nu} \int d\vec{r} \chi_{\nu}(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^{\pi}T(A-a,a)} \\
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&\stackrel{(a_{2\mu})}{\stackrel{I}{\longrightarrow}} \int d\vec{r} \begin{pmatrix} \alpha_{2\mu} \\ \alpha_{1\mu} + \alpha_{2\mu} + \alpha_{3\mu} = A \\ (M_{A}^{J^{\pi}T}) = \sum_{\lambda} c_{\lambda} |A_{\mu}^{J^{\pi}T}\rangle + \sum_{\nu} \int d\vec{r} \left(\sum_{\nu'} \int d\vec{r}' \mathcal{N}_{\nu\nu'}^{-\frac{1}{2}}(\vec{r}, \vec{r}') \bar{\chi}_{\nu'}(\vec{r}')\right) \hat{A} \Phi_{\nu\vec{r}}^{J^{\pi}T(A-a,a)} \\
&\stackrel{+}{\stackrel{I}{\longrightarrow}} \begin{pmatrix} H_{NCSM} & \cdots & \bar{h} \\ \bar{\chi} &= 1 + \nu + (a_{1}^{-1}) \begin{pmatrix} c \\ c \end{pmatrix} = E \begin{pmatrix} 1 & \bar{g} \\ 1 & \bar{g} \end{pmatrix} \begin{pmatrix} c \\ c \end{pmatrix}
\end{aligned}$$



Extending no-core shell model beyond bound states

Include more many nucleon correlations...

NCSM

$$\Psi^{A} = \sum_{n=0}^{N_{max}} \sum_{i} c_{Ni} \Phi_{Ni}^{A}$$

$$|\Psi_{A}^{J^{\pi}T}\rangle = \sum_{\nu} \int d\vec{r} \chi_{\nu}(\vec{r}) \hat{A} \Phi_{\nu\vec{r}}^{J^{\pi}T}(A-a,a)$$

$$(A) = \sum_{\lambda} \int d\vec{r} (A) = \sum_{\nu} \int d\vec{r} (A) = E \left(\int$$



Group

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

- No-core shell model (NCSM)
 - A-nucleon wave function expansion in the harmonicoscillator (HO) basis
 - short- and medium range correlations
 - Bound-states, narrow resonances
- NCSM with Resonating Group Method (NCSM/RGM)
 - cluster expansion, clusters described by NCSM
 - proper asymptotic behavior
 - Iong-range correlations
- Most efficient: *ab initio* no-core shell model with continuum (NCSMC)



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NCSM/RGM



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

Coupled NCSMC equations

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

$$\begin{bmatrix} E_{\lambda}^{NCSM} \delta_{\lambda\lambda'} & (A) & H \hat{A}_{\nu} | \stackrel{\vec{r}}{(a)} (A-a) \rangle \\ \downarrow & \downarrow \\ H_{NCSM} & h \\ \begin{pmatrix} H_{NCSM} & h \\ h \\ \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\ h \\ H_{RGM} \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\ \mathcal{O} \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & (A) & f \\ \delta_{\lambda\lambda'} & f \\ 1_{NCSM} & g \\ g \\ N_{RGM} \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\ \mathcal{O} \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\ g \\ g \\ N_{RGM} \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\ \mathcal{O} \end{pmatrix} | \begin{pmatrix} \mathcal{C} \\$$

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

Deuterium-Tritium fusion

- The $d^{+3}H \rightarrow n^{+4}He$ reaction
 - The most promising for the production of fusion energy in the near future
 - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
 - With its mirror reaction, ${}^{3}\text{He}(d,p){}^{4}\text{He}$, important for Big Bang nucleosynthesis







NCSMC calculation of the DT fusion

$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| \stackrel{^{5}\text{He}}{\bigoplus}, \lambda \right| + \int d\vec{r} \, u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \stackrel{\vec{r}}{\bigoplus} , \nu_{DT} \right| + \int d\vec{r} \, u_{\nu_{n\alpha}}(\vec{r}) \hat{A}_{n\alpha} \left| \stackrel{\vec{r}}{\bigoplus} , \stackrel{n}{\longleftarrow} , \nu_{n\alpha} \right|$$

- 2x7 static ⁵He eigenstates computed with the NCSM
- Continuous D-T(g.s.) cluster states (entrance channel)
 - Including positive-energy eigenstates of D to account for distortion
- Continuous n-⁴He(g.s.) cluster states (exit channel)
- Chiral NN+3N(500) interaction



n-⁴He scattering and ³H+d fusion within NCSMC





FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

⁴He

of $d+{}^{3}H$ is S-wave to $n+{}^{4}He$ in D-wave: Importance of the tensor and 3N force 14















Assuming the fusion proceeds only in S-wave with spins of D and T completely aligned: Polarized cross section 50% higher than unpolarized

While the DT fusion rate has been measured extensively, a standing of the process is still and in the standing of the

 Very little is known experimentally of now the polarization of the reactants' spins affects the reaction

$$\sigma_{unpol} = \sum_{J} \frac{2J+1}{(2I_{D}+1)(2I_{T}+1)} \sigma_{J}$$

$$\approx \frac{1}{3}\sigma_{1}^{2} + \frac{2}{3}\sigma_{3}^{3}$$

$$\sigma_{pol} \approx 1.5 \sigma_{unpol}$$



Polarized fusion

$$\frac{\partial \sigma_{pol}}{\partial \Omega_{c.m.}}(\theta_{\text{c.m.}}) = \frac{\partial \sigma_{unpol}}{\partial \Omega_{c.m.}}(\theta_{\text{c.m.}}) \left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta_{\text{c.m.}}) + \frac{3}{2}p_zq_zC_{z,z}(\theta_{\text{c.m.}})\right)$$



Ab initio predictions for polarized deuteriumtritium thermonuclear fusion

Guillaume Hupin^{1,2,3}, Sofia Quaglioni ³ & Petr Navrátil⁴

NCSMC calculation demonstrates impact of partial waves with l > 0as well as the contribution of l = 0 $J^{\pi} = \frac{1}{2}^{+}$ channel



Polarized fusion

$$\frac{\partial \sigma_{pol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) = \frac{\partial \sigma_{unpol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) \left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta_{c.m.}) + \frac{3}{2}p_zq_zC_{z,z}(\theta_{c.m.})\right)$$

 $10^{9}E$



$\neg 5 \cdot 10^{8}$ STORE STORE [] $N_{\rm A} \langle \sigma v \rangle^{-1} {\rm S. } \frac{10^8}{10^8} {\rm Gm}^3 {\rm Cm}^3 {\rm Im}^3 {\rm$ $5 \cdot 10^7$ $\substack{p_z=0.8,\; q_z=0.8\\p_{zz}=0.8}$ Unpolarized Bosch and Hale Descouvement NACRE $\overline{5 \cdot 10^{0}}$ 10^{1} $2 \cdot 10^1$ $5\cdot 10^1$ 10^{2} $2 \cdot 10^2$ $5 \cdot 10^{2}$ T [keV]

$$\langle \sigma \nu \rangle = \sqrt{\frac{8}{\pi \mu (k_b T)^3}} \int_0^\infty S(E) \exp\left(-\frac{E}{k_b T} - \sqrt{\frac{E_g}{E}}\right) dE,$$

For a realistic 80% polarization, reaction rate increases by ~32% or the same rate at ~45% lower temperature

ARTICLE https://doi.org/10.1038/s41467-018-08052-6 OPEN

Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

Neutron-rich halo nucleus¹¹Be

Z=4, N=7

- In the shell model picture g.s. expected to be J^π=1/2⁻
 - Z=6, N=7 ¹³C and Z=8, N=7 ¹⁵O have J^π=1/2⁻ g.s.
- In reality, ¹¹Be g.s. is J^π=1/2⁺ parity inversion
- Very weakly bound: E_{th}=-0.5 MeV
 - Halo state dominated by ¹⁰Be-n in the S-wave
- The 1/2⁻ state also bound only by 180 keV
- Can we describe ¹¹Be in *ab initio* calculations?
 - Continuum must be included
 - Does the 3N interaction play a role in the parity inversion?





Structure of ¹¹Be from chiral NN+3N forces

- NCSMC calculations including chiral 3N (N³LO NN+N²LO 3NF400, NNLOsat)
 - n-¹⁰Be + ¹¹Be
 - ¹⁰Be: 0⁺, 2⁺, 2⁺ NCSM eigenstates
 - ¹¹Be: $\geq 6 \pi = -1$ and $\geq 3 \pi = +1$ NCSM eigenstates



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



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



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Photo-disassociation of ¹¹Be

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

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

L. Moschini^{a,*}, P. Capel^{b,a}

Neutron transfer reactions in halo effective field theory

M. Schmidt,^{1,2} L. Platter,^{2,3} and H.-W. Hammer^{1,4} arXiv:1812.09152

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

C oss a

Halo sd-shell nucleus ¹⁵C and its unbound mirror ¹⁵F

• Motivation:

- Halo ½+ S-wave and 5/2+ D-wave bound states
- ${}^{14}C(n,\gamma){}^{15}C$ capture relevant for astrophysics
- Unbound ¹⁵F mirror very narrow unnatural parity resonances embedded in continuum predicted in ¹⁴O(p,p)¹⁴O
 - measured at GANIL
- Calculations in progress all results preliminary
- NN chiral interaction N³LO Entem & Machleidt 2003, SRG evolved with λ = 2.0 fm⁻¹
- 3N chiral interaction N²LO with local/non-local regulator, SRG evolved with λ = 2.0 fm⁻¹

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- NCSMC
 - ¹⁴C (¹⁴O) 0⁺ and 2⁺ eigenstates
 - ¹⁵C (¹⁵F) lowest 7 positive and 3 negative parity eigenstates

- NCSMC
 - ¹⁴C (¹⁴O) 0⁺ and 2⁺ eigenstates
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Table 15.1 from (1991AJ01): Energy levels of $^{15}\mathrm{C}\,^\mathrm{a}$

$E_{\rm x}~({\rm MeV}\pm{\rm keV})$	$J^{\pi}; T$	$ au$ or $\Gamma_{\rm c.m.}$ (keV)	Decay	Reactions
g.s.	$\frac{1}{2}^+; \frac{3}{2}$	$\tau_{1/2} = 2.449 \pm 0.005 \; \mathrm{s}$	β^{-}	1, 2, 3, 4, 6, 7, 9
		$ g = 2.63 \pm 0.14$		
0.7400 ± 1.5	$\frac{5}{2}^{+}$	$\tau_{\rm m}=3.76\pm0.10~{\rm ns}$	γ	2, 3, 4, 7, 8
		$g = -0.703 \pm 0.012$		
3.103 ± 4	$\frac{1}{2}^{-}$	$\Gamma_{\rm c.m.} \le 40$		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	$\left(\frac{5}{2}, \frac{7}{2}^+, \frac{9}{2}^+\right)$	< 20		2,3
6.417 ± 6	$\left(\frac{3}{2} \rightarrow \frac{7}{2}\right)$	≈ 50		2,3
6.449 ± 7	$(\frac{9}{2}^{-},\frac{11}{2})$	< 14		2,3
6.536 ± 4	а	< 14		2,3
6.626 ± 8	$(\frac{3}{2})$	20 ± 10		2,3
6.841 ± 4	а	< 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 $^{\rm b}$				2
8.01 ± 30				2

¹⁵C cluster form factors

- 1/2⁺ S-wave and 5/2⁺ D-wave ANCs
 - $C_{1/2+} = 1.282 \text{ fm}^{-1/2}$ compare to Moschini & Capel inferred from transfer data: 1.26(2) fm^{-1/2}
 - $C_{5/2+} = 0.048 \text{ fm}^{-1/2}$
 - Spectroscopic factors: 0.96 for 1/2⁺ and 0.90 for 5/2⁺ experiments 0.95(5) and 0.69, resp.

0.056(1) fm^{-1/2}

$^{14}C(n,\gamma)^{15}C$ capture cross section

Comparison to Karlsruhe experiment – Phys. Rev. C 77, 015804 (2008)

Conclusions

- *Ab initio* calculations of nuclear structure and reactions becoming feasible beyond the lightest nuclei
 - Make connections between the low-energy QCD, many-body systems, and nuclear astrophysics
- Polarized DT fusion investigated within NCSMC
 - Sheds light on importance of I>0 partial waves
- ¹¹Be parity inversion explained with chiral NN+3N N²LO_{sat} interaction
- NCSMC calculations of ¹⁵C sd-shell halo nucleus in progress
 - Capture cross section, cluster form factors, ANCs
- Study of the unbound ¹⁵F (mirror of ¹⁵C) in progress
 - Structure of resonances

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Thank you! Merci! Grazie!

