TRIUMF

Canada's national laboratory for particle and nuclear physics

Laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules

Electromagnetic transitions within the NCSMC

Jérémy Dohet-Eraly (TRIUMF)

Progress in Ab Initio Techniques in Nuclear Physics, TRIUMF, Vancouver, BC, Canada, February 24th, 2015.

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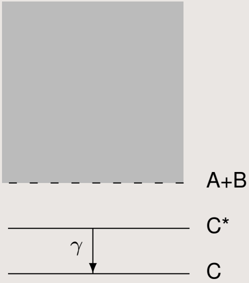
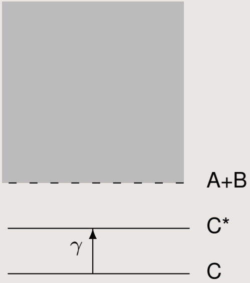
Electromagnetic transitions...

...between bound states...



Photoemission

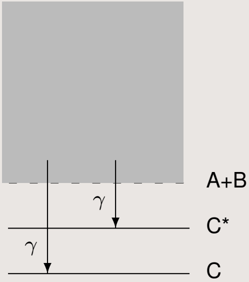


Photoabsorption

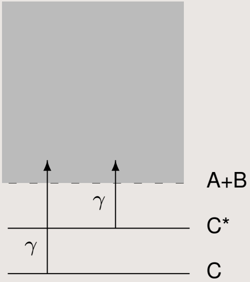
... to study the nuclear structure

Electromagnetic transitions...

...between a continuum state and a bound state...



Radiative capture

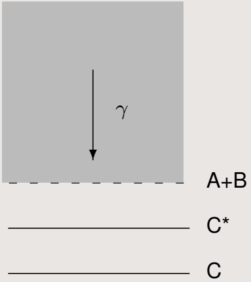


Photodisintegration

... to study the nuclear structure
... to understand the stellar nucleosynthesis

Electromagnetic transitions...

...between continuum states...



Nucleus-nucleus bremsstrahlung

... to study resonance spectra
... to diagnose thermonuclear burn

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Theoretical description

To describe these different transitions
we NEED

- Unified approach to describe bound and continuum states

$$\Rightarrow \Psi_{ini} \text{ and } \Psi_{fin}$$

We use the No-Core Shell Model with Continuum (NCSMC) approach

- Efficient way to calculate photoemission/photoabsorption matrix elements between bound states or bound and continuum states or continuum states

$$\Rightarrow \langle \Psi_{fin} | \mathcal{M}^{E}_{\lambda\mu} | \Psi_{ini} \rangle$$

Starting point

Microscopic Schrödinger equation

$$\left(\sum_{i=1}^{A}\frac{p_i^2}{2m_N}+\sum_{i>j=1}^{A}v_{ij}+\sum_{i>j>k=1}^{A}v_{ijk}-T_{\rm c.m.}\right)|\Psi_A^{J^\pi T}\rangle = E|\Psi_A^{J^\pi T}\rangle$$

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kinetic energy
of nucleon *i*

Starting point

Microscopic Schrödinger equation

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kinetic energy
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chiral NN (+3N) interactions
softened by the
similarity renormalization group method

D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001 (2003)
P. Navrátil, Few-Body Syst. 41, 117 (2007)
S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C 75, 061001 (2007)

Starting point

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kinetic energy of nucleon i

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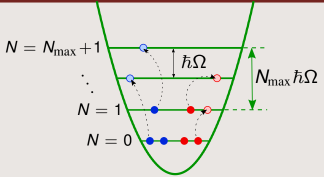
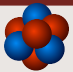
No-core shell model with continuum w.f.

No-core shell model with continuum



No-core shell model (NCSM)



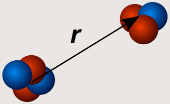
- Slater determinants of harmonic oscillator functions
- Exact c.m. factorization
- Short- and medium-range correlations
- Bound-state method

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J\pi T} \underbrace{|\ \rangle}_{\textit{NCSM}}$$

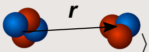
No-core shell model with continuum

+NCSM/resonating group method (RGM)

- Clustering; Long-range correlations
- Bound and scattering states; reactions



$$|\Psi_A^{J^\pi T}\rangle = \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J^\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\ \rangle}_{NCSM\,/\,RGM}$$



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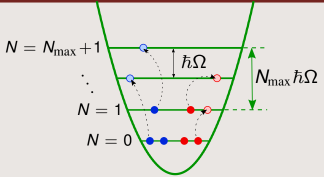
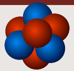


No-core shell model (NCSM)



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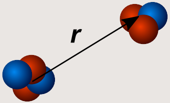
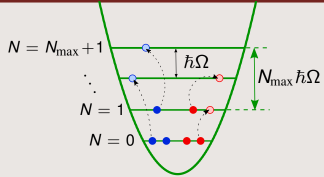


= No-core shell model with continuum

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

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda^{J\pi T} \underbrace{|\;\rangle}_{NCSM} + \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\;\rangle}_{NCSM\,/\,RGM}$$

No-core shell model with continuum



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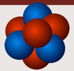

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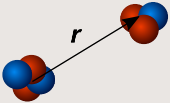

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$$+ \sum_\nu \int dr\, r^2 \frac{\gamma_\nu^{J\pi T}(r)}{r} \mathcal{A}_\nu \underbrace{|\;\cdot\;\rangle}_{NCSM\,/\,RGM}$$

unknowns

NCSMC equations

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda \underbrace{c_\lambda^{J^\pi T}}_{unknown} |\;\rangle + \sum_\nu \int dr\, r^2 \underbrace{\frac{\gamma_\nu^{J^\pi T}(r)}{r}}_{unknown} \mathcal{A}_\nu |\;\overset{r}{\longrightarrow}\;\rangle$$

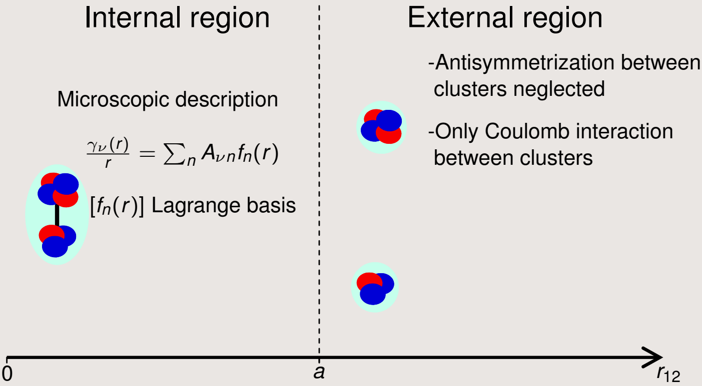
- Variational amplitudes ($c_\lambda^{J^\pi T}$ and $\gamma_\nu^{J^\pi T}$) obtained by solving the NCSMC equations

$$\begin{pmatrix} E_\lambda \delta_{\lambda\lambda'} & \langle\;|H\mathcal{A}_\nu|\;\overset{r}{\longrightarrow}\;\rangle \\ \langle\;\overset{r}{\longrightarrow}\;|\mathcal{A}_{\nu'} H|\;\rangle & \langle\;\overset{r}{\longrightarrow}\;|\mathcal{A}_{\nu'} H \mathcal{A}_\nu|\;\overset{r}{\longrightarrow}\;\rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} \delta_{\lambda\lambda'} & \langle\;|\mathcal{A}_\nu|\;\overset{r}{\longrightarrow}\;\rangle \\ \langle\;\overset{r}{\longrightarrow}\;|\mathcal{A}_{\nu'}|\;\rangle & \langle\;\overset{r}{\longrightarrow}\;|\mathcal{A}_{\nu'} \mathcal{A}_\nu|\;\overset{r}{\longrightarrow}\;\rangle \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

- Most challenging: calculation of kernels (mostly due to $\mathcal{A}_\nu$)
- Scattering matrix and asymptotic normalization coefficients from matching solutions to known asymptotic with coupled-channel microscopic *R*-matrix method (MRM) on Lagrange mesh

  [M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]

MRM on a Lagrange mesh



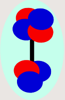
[D. Baye, P.-H. Heenen, and M. Libert-Heinemann, Nucl. Phys. A 291 (1977) 230]
[M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]
[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]

MRM on a Lagrange mesh

Internal region

Microscopic description

$\frac{\gamma_\nu(r)}{r} = \sum_n A_{\nu n} f_n(r)$



$[f_n(r)]$ Lagrange basis

External region

-Antisymmetrization between clusters neglected

-Only Coulomb interaction between clusters

$\Rightarrow \gamma_\nu(r) \propto C_\nu W(k_\nu r)$ (bound state)

$\propto \delta_{\nu i} I_\nu(k_\nu r) - U_{\nu i} O_\nu(k_\nu r)$ (scattering state)

$\propto O_\nu(k_\nu r)$ (resonance)

0   a r_{12}

[D. Baye, P.-H. Heenen, and M. Libert-Heinemann, Nucl. Phys. A 291 (1977) 230]
[M. Hesse, J.-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. A 640, 37 (1998)]
[P. Descouvemont and D. Baye, Rep. Prog. Phys. 73 (2010) 036301]

Electric transitions

$$|\Psi_A^{J^\pi T}\rangle = \sum_\lambda c_\lambda |$$  $$\rangle + \sum_\nu \int dr\, r^2 \frac{\gamma_\nu(r)}{r} \mathcal{A}_\nu |$$  $$\rangle$$

Schematically

$$\langle \Psi_f^{J'\pi' T'} || \mathcal{M}_\lambda^E || \Psi_i^{J\pi T}\rangle = \sum_{\lambda\lambda'} c_{\lambda'}^* c_\lambda \langle \Phi_{\lambda'} || \mathcal{M}_\lambda^E || \Phi_\lambda \rangle + \sum_{\lambda\nu'} c_\lambda \int dr\, r^2 \frac{\gamma_{\nu'}'^*(r)}{r} \langle \Phi_{r} || \mathcal{A}_{\nu'} \mathcal{M}_\lambda^E || \Phi_\lambda \rangle$$
$$+ \sum_{\lambda'\nu} c_{\lambda'}^* \int dr\, r^2 \frac{\gamma_\nu(r)}{r} \langle \Phi_{\lambda'} || \mathcal{M}_\lambda^E \mathcal{A}_\nu || \Phi_{r} \rangle$$
$$+ \sum_{\nu\nu'} \iint dr\, dr'\, r^2 r'^2 \frac{\gamma_{\nu'}'^*(r)}{r} \frac{\gamma_\nu(r)}{r} \langle \Phi_{r} || \mathcal{A}_{\nu'} \mathcal{M}_\lambda^E \mathcal{A}_\nu || \Phi_{r} \rangle$$

When a RGM state is included, use of

$$\mathcal{M}_{\lambda\mu}^E \approx \mathcal{M}_{\lambda\mu}^E(1) + \mathcal{M}_{\lambda\mu}^E(2) + e\left[Z_1\left(\frac{A_2}{A}\right)^\lambda + Z_2\left(\frac{-A_1}{A}\right)^\lambda\right] r_{12}^\lambda Y_{\lambda\mu}(\hat{r}_{12})$$

Exact for *E*1 transitions!

Electric transitions

Trick for relative term:

$$r_{12}^{\lambda} Y_{\lambda\mu}(\hat{r}_{12}) \mathcal{A}_{\nu} | \overset{r}{\longrightarrow}; \nu \rangle = r_{12}^{\lambda} \sum_{\tilde{\nu}} d_{\nu\tilde{\nu}} \mathcal{A}_{\tilde{\nu}} | \overset{r}{\longrightarrow}; \tilde{\nu} \rangle$$

For $\mathcal{M}^{E}_{\lambda\mu}(1)$ and $\mathcal{M}^{E}_{\lambda\mu}(2)$, use of closure relation

$$\langle \overset{r}{\longrightarrow}; \nu' || \mathcal{A}_{\nu'} \mathcal{A}_{\nu} \mathcal{M}^{E}_{\lambda}(1) || \overset{r}{\longrightarrow}; \nu \rangle = \sum_{\tilde{\nu}} \langle \overset{r}{\longrightarrow}; \nu' | \mathcal{A}_{\nu'} \mathcal{A}_{\nu} | \overset{r}{\longrightarrow}; \tilde{\nu} \rangle \langle \overset{r}{\longrightarrow}; \tilde{\nu} || \mathcal{M}^{E}_{\lambda}(1) || \overset{r}{\longrightarrow}; \nu \rangle$$

Electric transitions

Trick for relative term:

$$r_{12}^{\lambda} Y_{\lambda\mu}(\hat{r}_{12}) \mathcal{A}_{\nu} | \; r \; ; \nu \rangle = r_{12}^{\lambda} \sum_{\tilde{\nu}} d_{\nu\tilde{\nu}} \mathcal{A}_{\tilde{\nu}} | \; r \; ; \tilde{\nu} \rangle$$

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Good news

Electric transitions

Trick for relative term:

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Good news

- Electromagnetic matrix elements deduced from overlap NCSMC matrix elements and NCSM matrix elements

Electric transitions

Trick for relative term:

$$r_{12}^{\lambda} Y_{\lambda\mu}(\hat{r}_{12}) \mathcal{A}_{\nu} |\overset{r}{\bullet\!-\!\bullet}; \nu\rangle = r_{12}^{\lambda} \sum_{\tilde{\nu}} d_{\nu\tilde{\nu}} \mathcal{A}_{\tilde{\nu}} |\overset{r}{\bullet\!-\!\bullet}; \tilde{\nu}\rangle$$

For $\mathcal{M}^{E}_{\lambda\mu}(1)$ and $\mathcal{M}^{E}_{\lambda\mu}(2)$, use of closure relation

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Good news

- Electromagnetic matrix elements deduced from overlap NCSMC matrix elements and NCSM matrix elements
- Overlap NCSMC matrix elements already calculated for getting the bound and scattering states

Radiative captures

Reactions

Motivations

Extra motivation

Radiative captures

Reactions

- $^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$ and $^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$

Motivations

Extra motivation

Radiative captures

Reactions

- $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ and $^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$

Motivations

- calculate the primordial $^7\mathrm{Li}$ abundance in the universe
- input for standard solar models to determine the fraction of pp-chain branches resulting in $^7\mathrm{Be}$ versus $^8\mathrm{B}$ neutrinos

Extra motivation

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Radiative captures

Reactions

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- Coulomb barrier strongly suppresses the capture cross sections $\Rightarrow$ at low energies out of reach of the experiments

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Extra motivation

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[J D-E, P. Navrátil, S. Quaglioni, W. Horiuchi, G. Hupin, F. Raimondi, arXiv:1510.07717 [nucl-th]]

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^{7}Be and ^{7}Li bound-state properties

	^{7}Be			^{7}Li		
	NCSM	NCSMC	Exp	NCSM	NCSMC	Exp
$E_{3/2-}$ (MeV)	-0.82	-1.52	-1.587	-1.79	-2.43	-2.467
$E_{1/2-}$ (MeV)	-0.49	-1.26	-1.157	-1.46	-2.15	-1.989
$r_{\rm ch}$ (fm)	2.375	2.62	2.647(17)[a]	2.21	2.42	2.39(3)[b]
Q (e fm^2)	-4.57	-6.14		-2.67	-3.72	-4.00(3)[c]
μ (μ_N)	-1.14	-1.16	-1.3995(5)[a]	3.00	3.02	3.256[d]

[a] W. Nortershauser *et al.*, Phys. Rev. Lett. 102 (2009) 062503

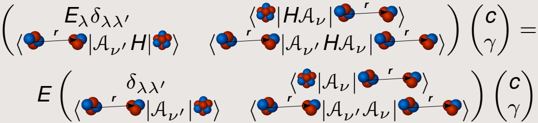
[b] C. D. Jager, H. D. Vries, and C. D. Vries, Atom. Data Nucl. Data 14 (1974) 479

[c] H.-G. Voelk and D. Fick, Nucl. Phys. A 530 (1991) 475

[d] P. Raghavan, Atom. Data Nucl. Data 42 (1989) 189

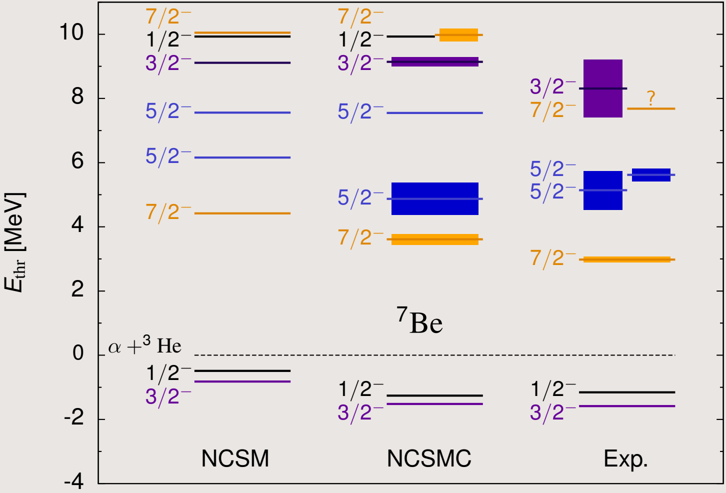
Phenomenological NCSMC

- NCSMC equations

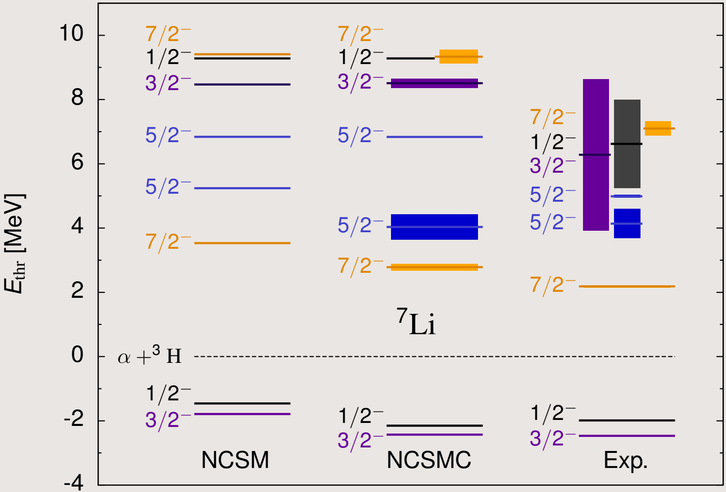


- Considering E_λ as adjustable parameters to reproduce the bound-state and resonance energies

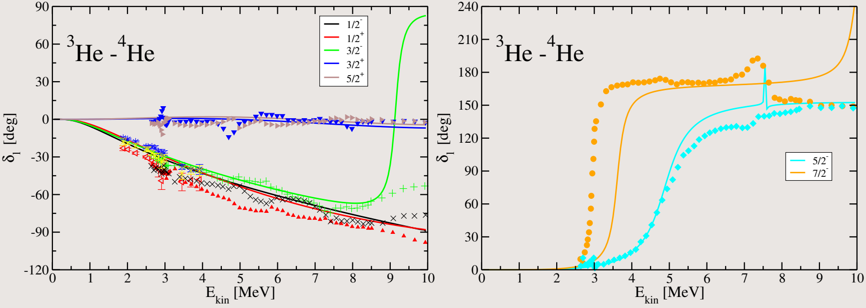
^{7}Be spectrum



^{7}Li spectrum



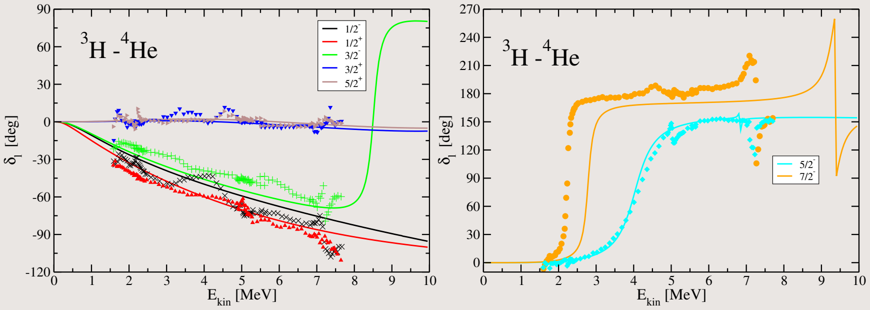
$\alpha + ^3$ He phase shifts



- NCSMC calculations with SRG N^{3}LO *NN* potential ($\lambda = 2.15$ fm^{-1})
- $N_{max} = 12; \hbar\Omega = 20$ MeV ; ^{3}He, α ground state
- 8 (6) eigenstates with negative (positive) parity of ^{7}Be

Nota: Recent $\alpha + ^3$ He elastic cross sections measurements at TRIUMF. Analysis in progress.

$\alpha +^3$ H phase shifts



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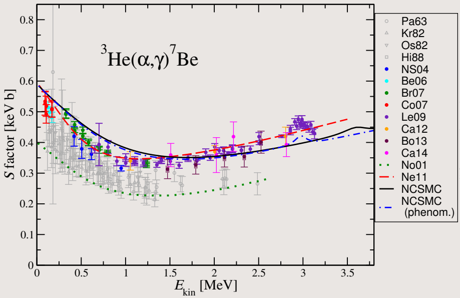
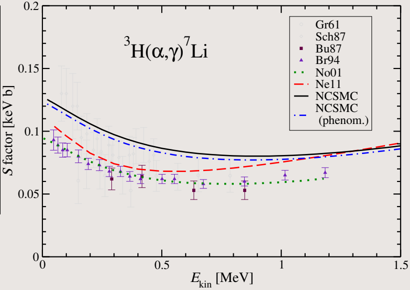
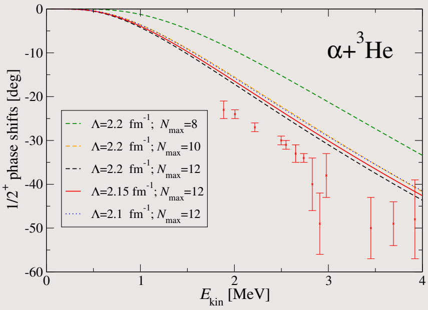
$^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$





$\alpha + ^3$He phase shifts



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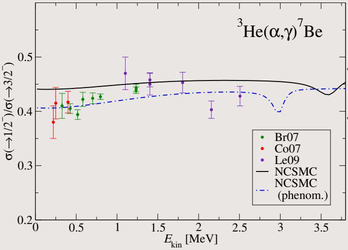
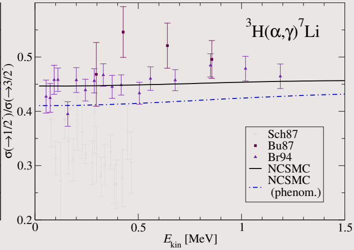
$^3He(\alpha,\gamma)^7Be$ and $^3H(\alpha,\gamma)^7Li$

"Branching ratio"





Photodisintegration

Reaction

Motivations

Photodisintegration

Reaction

- $^11\mathrm{Be} + \gamma \rightarrow {}^{10}\mathrm{Be} + n$

Motivations

Photodisintegration

Reaction

- $^11\mathrm{Be} + \gamma \rightarrow {}^{10}\mathrm{Be} + n$

Motivations

- Parity inversion of the two bound states with respect to the shell model predictions

TRIUMF

Photodisintegration

Reaction

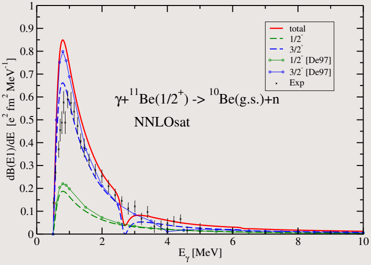
- $^{1}1\mathrm{Be} + \gamma \rightarrow {}^{10}\mathrm{Be} + n$

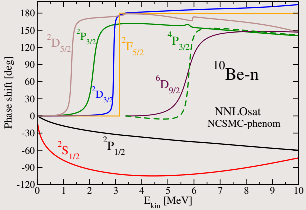
Motivations

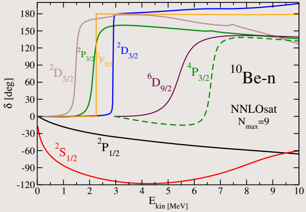
- Parity inversion of the two bound states with respect to the shell model predictions
- one-neutron halo nucleus

^{11}Be photodisintegration

Preliminary!





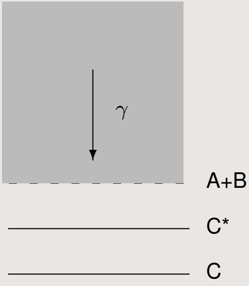


NNLO$_{sat}$, $\hbar\Omega = 20$ MeV

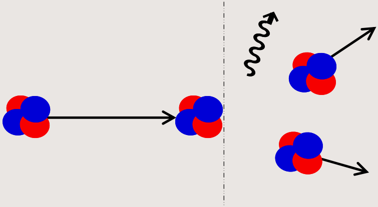
Cluster-model results from [De97] P. Descouvemont, Nucl. Phys. A 615 (1997) 261.

Exp. data from R. Palit *et al.*, Phys. Rev. C 68 (2003) 034318.

Nucleus-nucleus bremsstrahlung



Nucleus-nucleus bremsstrahlung



- photon emission induced by a collision between two nuclei
- Part of the collision energy converted to a photon

Bremsstrahlung

Motivations

- to describe the radiative transitions between unstable states
  - Recent measurements of "4^+-to-2^+" gamma transitions in $^8\mathrm{Be}$ from the $\alpha(\alpha, \alpha\alpha\gamma)$ performed at Mumbai (India).
    [V. M. Datar *et al.*, PRL 94 (2005) 122502] [V. M. Datar *et al.*, PRL 111 (2013) 062502]

- to describe the $t(d, n\gamma)\alpha$ radiative transfer reaction
  - perspective to diagnose plasmas in fusion experiments from this reaction
  - recent experiment at University of Rochester and at Ohio university
    [Y. Kim *et al.*, PRC 85 (2012) 061601(R)]

- to describe the $\alpha + N \rightarrow \alpha + N + \gamma$ reaction
  - Possible comparison with experiment for the $\alpha + p$ bremsstrahlung
  - Preliminary step to $t(d, n\gamma)\alpha$

Special features

From a continuum state to a continuum state!

- $\Rightarrow$ All partial waves need to be involved
  - For each multipole, selection rules restrict only the final state.
  - At low scattering angles and/or low photon energies, high partial wave play a significant role $\Rightarrow$ low convergent series (solution: Kummer's series transformation [Baye *et al.*, Nucl. Phys. A 529 (1991) 467])

- Two nuclei and one photon in the final channel $\Rightarrow$ more complicated kinematics

- Matrix elements of the electric operators diverge!

Divergence problem

- Electric operators

$$E_\lambda \underset{\rho\to\infty}{\longrightarrow} eZ_{\text{eff}}\rho^\lambda Y_\lambda(\Omega_\rho)$$

- Integrand

$$\Psi_f(E_f)E_\lambda\Psi_i(E_i) \propto \underbrace{\left[F_{l_f}(\rho)\cos\delta_{l_f} + G_{l_f}(\rho)\sin\delta_{l_f}\right]}_{\text{non}-\text{decreasing oscillating function}} \rho^\lambda \underbrace{\left[F_{l_i}(\rho)\cos\delta_{l_i} + G_{l_i}(\rho)\sin\delta_{l_i}\right]}_{\text{non}-\text{decreasing oscillating function}}$$

- $\Rightarrow$ divergence

Divergence problem

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- $\Rightarrow$ divergence
- Origin: $eZ_{\text{eff}}\rho^\lambda Y_\lambda(\Omega_\rho)$ (commonly used) is not the EXACT electric operator but a Siegert version based on the long-wavelength approximation ($k_\gamma r \ll 1$) but $r = \infty$ for a continuum state (in a stationary approach)

Divergence problem

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- Solution: use of an extended Siegert theorem valid at all photon energies

[K.-M. Schmitt, P. Wilhelm, H. Arenhövel, A. Cambi, B. Mosconi, and P. Ricci, Phys. Rev. C 41, 841 (1990)]
[JDE, D. Baye, Phys. Rev. C 88 (2013) 024602]
[JDE, Phys. Rev. C 89 (2014) 024617]
[JDE, D. Baye, Phys. Rev. C 90, (2014) 034611]

Electric operators

- Approximation: charge and current densities for free nucleons
- The Siegert electric transition multipole operators are given explicitly by

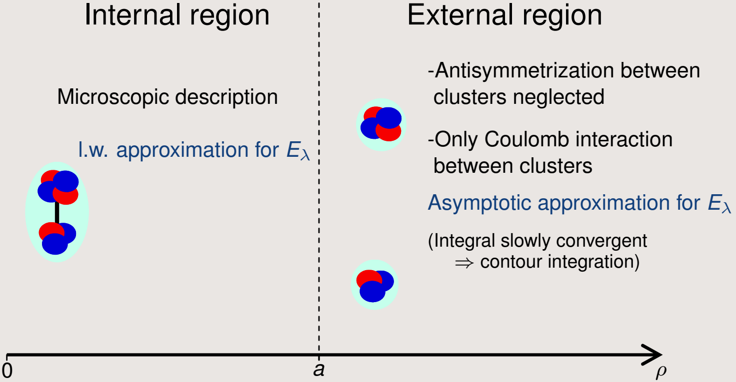
$$
\begin{aligned}
E_{\lambda\mu} = & \frac{e(2\lambda+1)!!}{k_\gamma^\lambda} \sum_{j=1}^{A} \left(\frac{1}{2} - t_{j3}\right) \phi_{\lambda\mu}\left[k_\gamma\left(\boldsymbol{r}_j - \boldsymbol{R}_{\mathrm{c.m.}}\right)\right] \\
& + \frac{ie(2\lambda+1)!!}{2m_N c(\lambda+1)k_\gamma^{\lambda+1}} \sum_{j=1}^{A} \Bigg\{ \left(\frac{1}{2} - t_{j3}\right) \\
& \left[\chi_{\lambda\mu}(k_\gamma, \boldsymbol{r}) - (\lambda+1)\boldsymbol{\nabla}\phi_{\lambda\mu}(k_\gamma \boldsymbol{r}), \boldsymbol{p}_j - A^{-1}\boldsymbol{P}_{\mathrm{c.m.}}\right]_+ \\
& - k_\gamma^2 g_{sj} (\boldsymbol{r} \times \boldsymbol{\nabla})\phi_{\lambda\mu}(k_\gamma \boldsymbol{r}) \cdot \boldsymbol{s}_j \Bigg\}_{\boldsymbol{r}=\boldsymbol{r}_j - \boldsymbol{R}_{\mathrm{c.m.}}} .
\end{aligned}
$$

where $[\boldsymbol{a}, \boldsymbol{b}]_+$ is a shorthand notation for $\boldsymbol{a} \cdot \boldsymbol{b} + \boldsymbol{b} \cdot \boldsymbol{a}$, g_{sj} is the gyromagnetic factor, and

$$
\chi_{\lambda\mu}(k_\gamma, \boldsymbol{r}) = \left(k_\gamma^2 \boldsymbol{r} + \boldsymbol{\nabla} \frac{\partial}{\partial r} r\right) \phi_{\lambda\mu}(k_\gamma \boldsymbol{r}),
$$

$$
\phi_{\lambda\mu}(k_\gamma \boldsymbol{r}) = j_\lambda(k_\gamma r) Y_{\lambda\mu}(\Omega).
$$

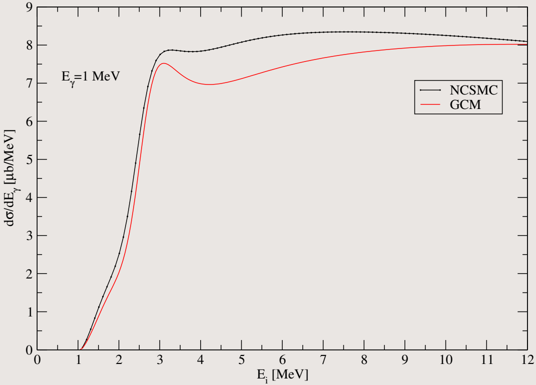
Microscopic *R*-Matrix on a Lagrange mesh



Approximations checked by varying a

$\alpha + p$ bremsstrahlung

Preliminary!



N3LO (EM) NN, N2LO(500) 3NF, $\lambda = 2\ \mathrm{fm}^{-1}$,$N_{\mathrm{max}} = 7$, $\hbar\Omega = 20\ \mathrm{MeV}$

[GCM] JDE, Phys. Rev. C 89 (2014) 024617

Conclusion

Summary

- No-Core Shell model with Continuum is extended to the description of electromagnetic transitions
- Current applications: ${}^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$ and ${}^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$ radiative captures, ${}^{11}\mathrm{Be}$ photodisintegration, and $\alpha + N$ bremsstrahlung
- Importance to reproduce the experimental thresholds and resonances
  - $\Rightarrow$ importance of three-nuclen forces
  - $\Rightarrow$ NCSMC phenomenological

Outlook

- Include three-nucleon forces
- Other applications: ${}^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$, $t(d,n\gamma)\alpha$, ...

Thank you!

Merci

Collaborators

- P. Navrátil (TRIUMF)
- G. Hupin (CEA)
- S. Quaglioni (LLNL)
- W. Horiuchi (Hokkaido University)
- F. Raimondi (University of Surrey)
- A. Calci (TRIUMF)