Cross sections of light-ion reactions calculated from *ab initio* wave functions

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In collaboration with:
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Nuclei in the Cosmos (NIC-IX),
CERN, Geneva, June 29, 2006

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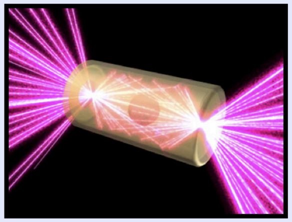
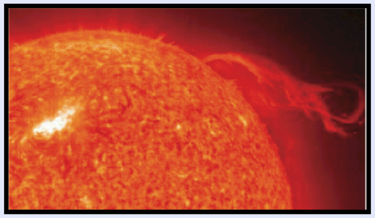
Low-energy, light-ion reactions

- **Underlying theory:** Non-relativistic quantum mechanics of many interacting nucleons
- Only a **few reaction channels** are important
- **Applications:** nuclear astrophysics, thermonuclear fusion





Potential-model description

- Dynamics of interacting nuclei described by simple local potentials

First-principles microscopic approach

- Fully antisymmetrized many-nucleon wave functions
- Realistic interactions between the nucleons

The microscopic *ab initio* approach

Aiming for truly predictive power…

Nuclear physicists now have access to:

- **State-of-the-art nuclear Hamiltonians**
  - Can either have roots in QCD or be based on traditional meson-exchange theory
  - Empirical in that they accurately fit a wealth of *NN* scattering data
- **State-of-the-art nuclear many-body methods**
  - A few methods are available for A>4 with the use of realistic interactions
- **State-of-the-art computing facilities**

The *ab initio* no-core shell model

• It is a general approach for studying strongly interacting, quantum many-body systems.

• It has been applied with great success to nuclear systems,
- with *NN* as well as *3N* interactions
- using local, as well as non-local potentials
- up to *A=20* (in smaller model spaces)

• A matrix diagonalization technique to solve the translational invariant A-body problem in a finite harmonic oscillator basis

• Basis truncation defined by the total number of oscillator quanta excitations ($\leq N_{max} h\Omega$) for the A particles

• Unitary transformation of the bare Hamiltonian performed to compute model-space dependent effective interaction

See, e.g., P. Navrátil, *et al*, Phys. Rev. C 62, 054311 (2000).

"Taking the model out of the shell model"

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Cluster overlap functions from NCSM wave functions

We can characterize the weight of a particular cluster component of a full A-body eigenstate by cluster overlap functions:

$$g_\nu(\vec{r}) = \left\langle \Phi_\nu^{(A)}(\vec{r}) \middle| \Psi^{(A)} \right\rangle$$ where $$\Phi_\nu^{(A)}(\vec{r}) = \mathcal{A}_\nu \left\{ \Phi_{1\nu} \Phi_{2\nu} \delta(\vec{r}_\nu - \vec{r}) \right\}$$

$$S_\nu = \int d^3r |g_\nu(\vec{r})|^2$$ - "Spectroscopic factor" $\Rightarrow$ coefficients of parentage

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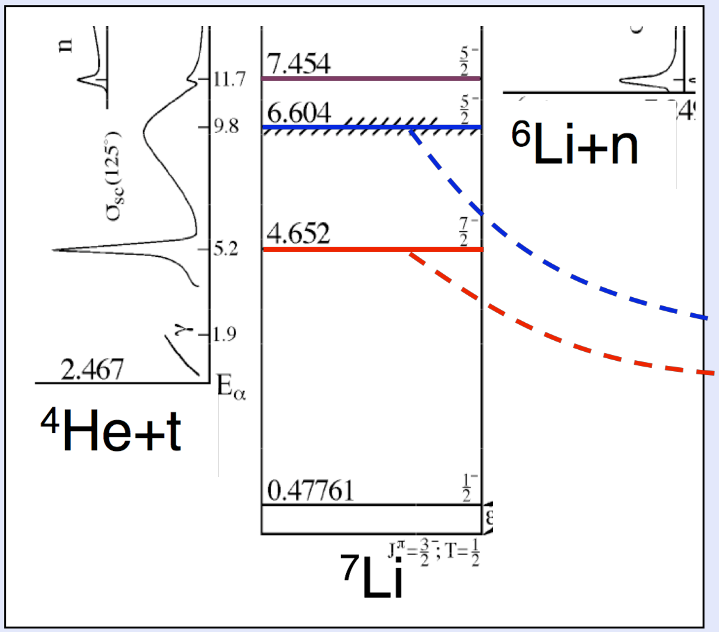
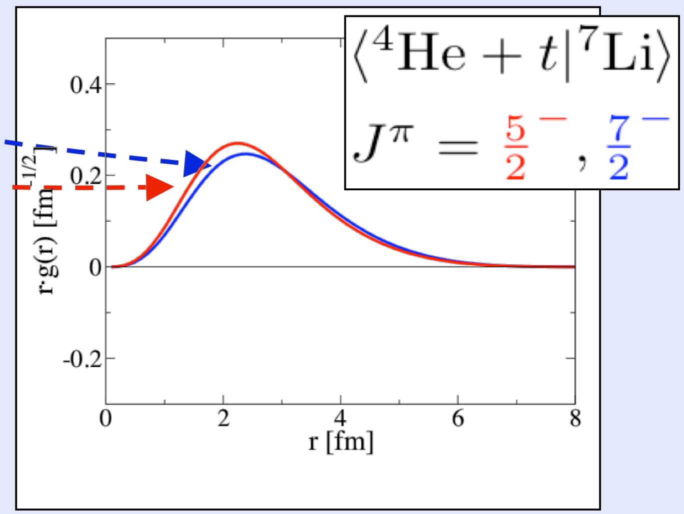


Example: How much do the states in ^{7}Li look like ^{4}He+t ?



P. Navrátil, Phys. Rev. C. **70**(2004)054324

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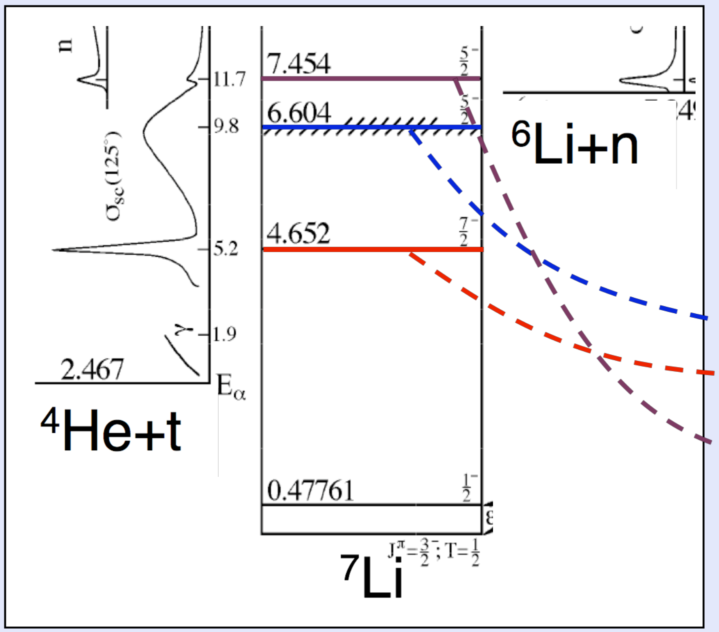

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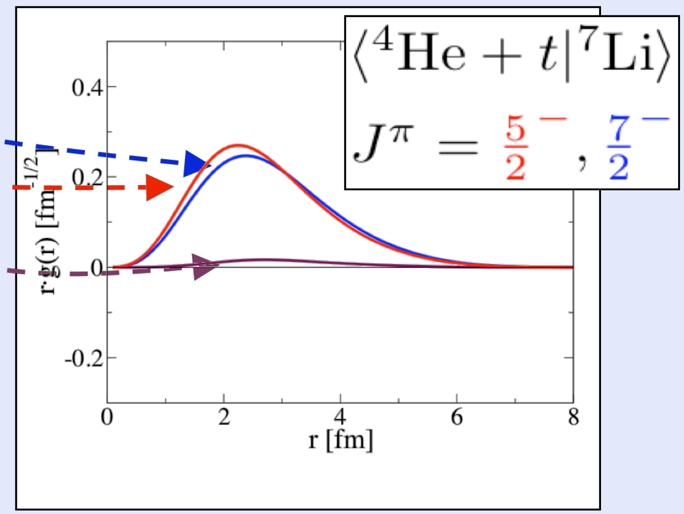

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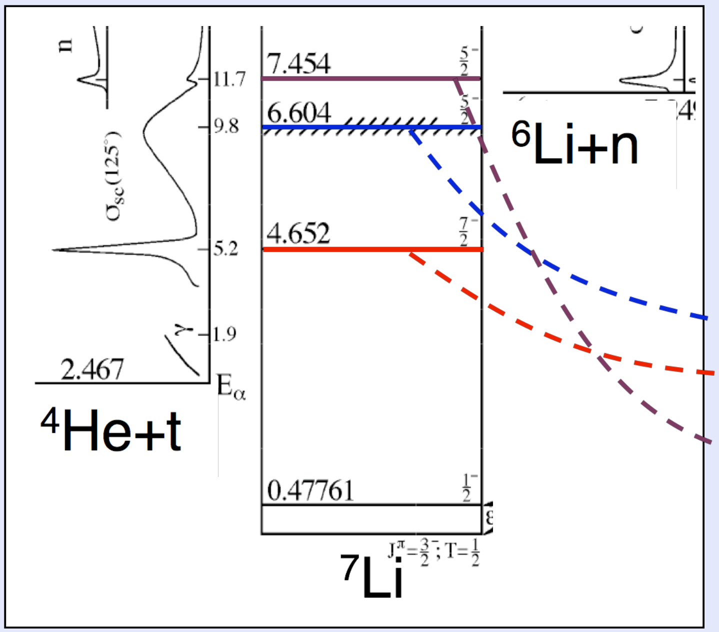

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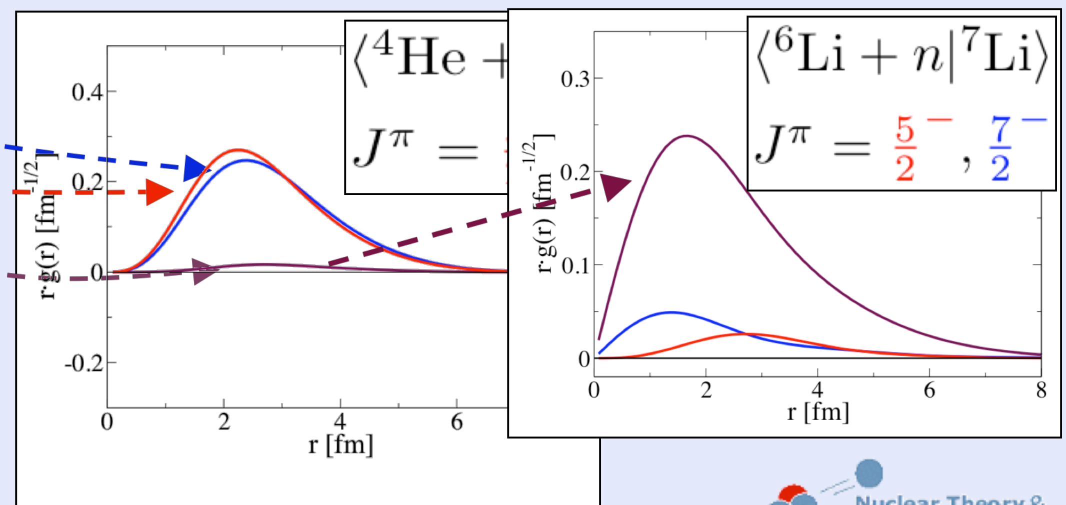
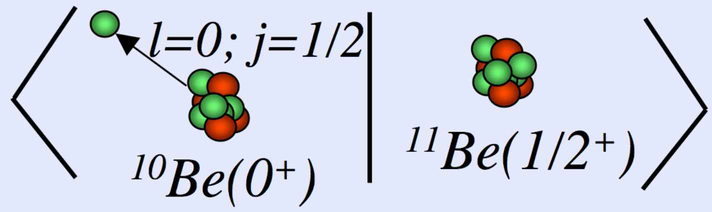


P. Navrátil, Phys. Rev. C. **70**(2004)054324

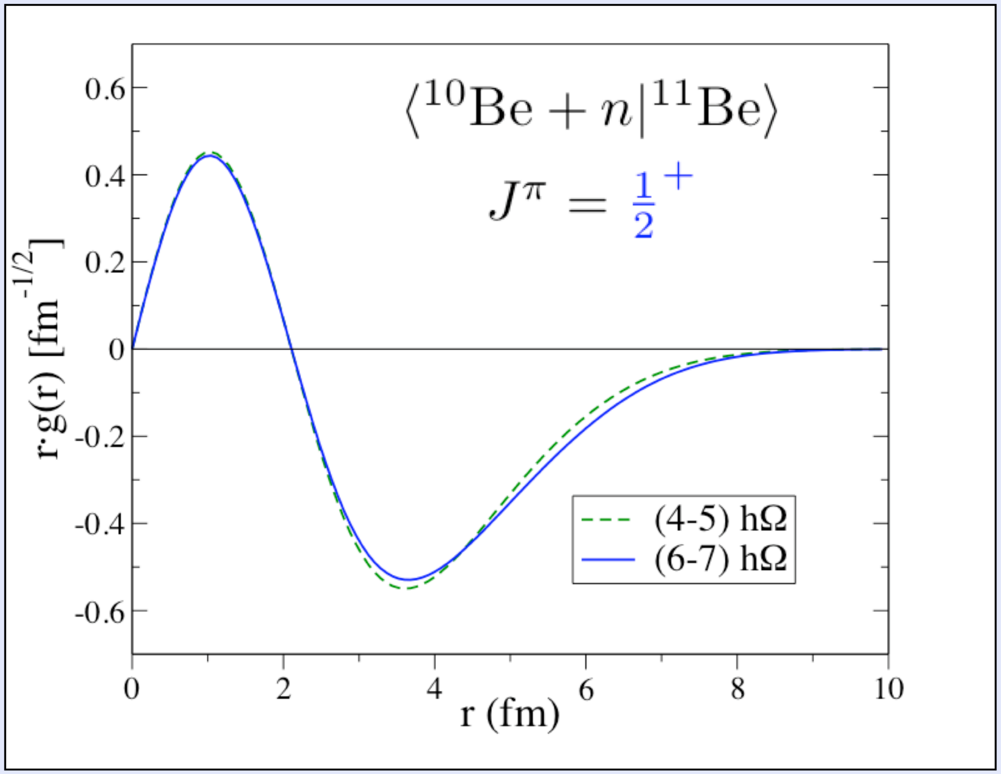
Next example: how much does $^{11}Be_{gs}$ look like $^{10}Be_{gs}$+n ?

Large-scale NCSM calculations with convergence tests for several A=9-13 isotopes

C. Forssén *et al*, Phys. Rev. C 71 (2005) 044312



Model space	Spec. factor
(4-5)hΩ	0.831
(6-7)hΩ	0.818



CD-Bonn 2000

$\hbar\Omega = 14$ MeV

$(4-5), (6-7)\hbar\Omega$

- Pauli principle inherent
- Stable spectroscopic factor
- Stable interior
- Incorrect asymptotics

C. Forssén, NIC-IX, CERN, Geneva, June 29, 2006

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Radiative capture cross sections

Electromagnetic transition probability from 1st order perturbation theory

$$T_{\mathrm{fi}} = \frac{2\pi}{\hbar^2} \left| \left\langle \Psi_f^{(A)} \left| H_{\mathrm{int}} \right| \Phi_i^{(A)} \right\rangle \right|^2$$

Using *ab initio* structure information:

- Final (bound) A-body state, as well as projectile and target eigenstates are obtained from NCSM.
- Cluster overlaps calculated for a few relevant two-body channels.
- Spectroscopic factors equals the integrals of the cluster overlaps.
- **Supplemental input:**
- Scattering wave function.
- Experimental threshold energies (see next slide).

Having a physically accurate picture is very important

- **Asymptotic behaviour:**

HO single-particle basis states

$$\varphi_{nlm}(r) \sim \exp\left(-r^2/b^2\right)$$

Physical bound-state wave function

$$u(r) \sim \exp\left(-\kappa_0 r\right)/r$$

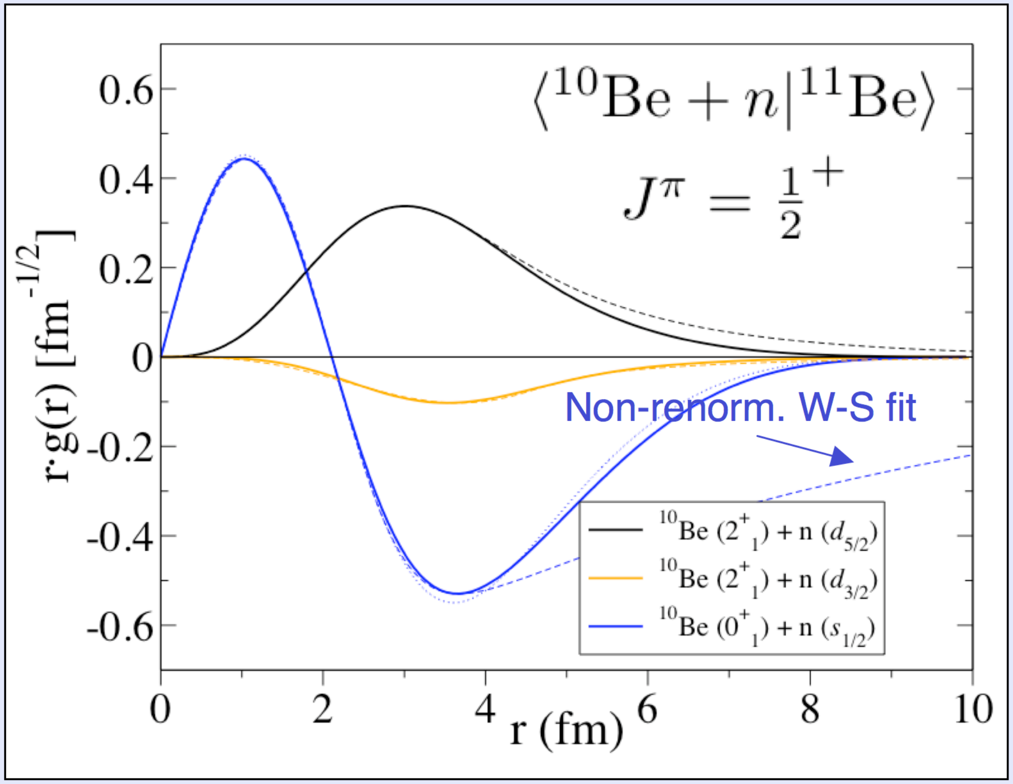
where $\kappa_0 \propto \sqrt{E_0}$

- **Construct effective inter-fragment potentials *$V_{eff}(r)$***

$$\boxed{\left[T + V_{\text{eff}} - E_0\right] u(r) = 0}$$

Exp. treshold energy

- **Renormalize the solution by NCSM spectroscopic factor**



$\mathrm{CD-Bonn}\ 2000$

$\hbar\Omega = 14\ \mathrm{MeV}$

$(6-7)\hbar\Omega$

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Results, inhomogeneous BB scenarios: $^{10}Be(n,\gamma)^{11}Be$

Suggestion: Inhomogenities in the distribution of baryons during the primordial nucleosynthesis can lead to the production of heavy elements.

See, e.g., T. Rauscher et al., Ap. J. **429**(1994)499

- $^{7}Li(n,\gamma)^{8}Li(\alpha,n)^{11}B(n,\gamma)^{12}B(\beta^{-})^{12}C(n,\gamma)^{13}C(n,\gamma)^{14}C(n,\gamma)^{15}C$ …
- $^{7}Li(n,\gamma)^{8}Li(n,\gamma)^{9}Li(\beta^{-})^{9}Be(n,\gamma)^{10}Be(n,\gamma)^{11}Be(\beta^{-})^{11}B(n,\gamma)^{12}B(\beta^{-})^{12}C(n,\gamma)$ …

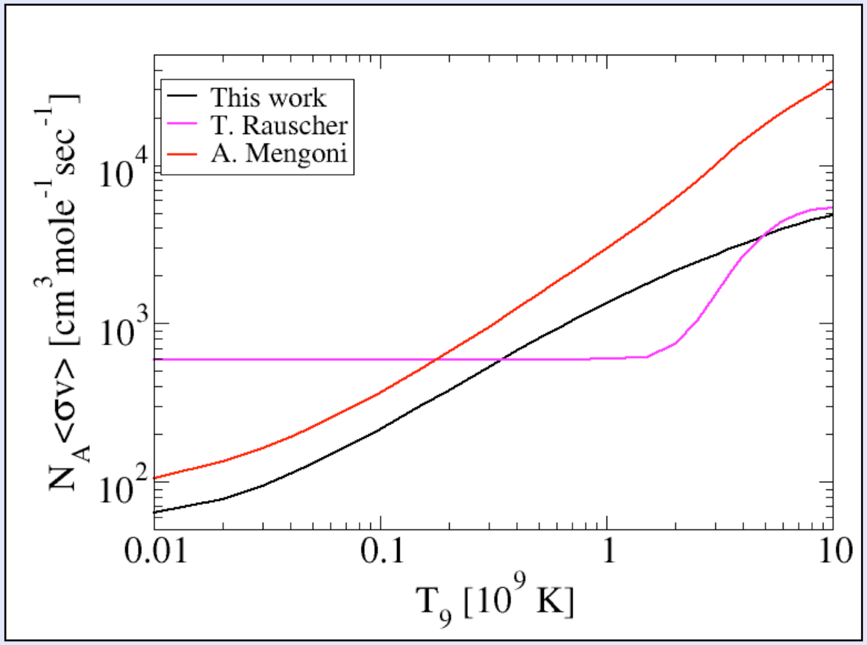
Study of $^{10}Be(n,\gamma)^{11}Be$:

• Cluster overlaps of bound states fitted in the 0-4 fm range. Model spaces up to 7hΩ

• Scattering states calculated from the same potentials.

• Our result updates two earlier estimates:
1. p-wave capture dominates
2. Resonant capture is negligible

• Most likely confirm the conclusion that $^{8}Li(\alpha,n)^{11}B$ is the relevant bottleneck in the IBBN reaction network.



Results, solar pp chain: ^{7}Be(p,γ)^{8}B

SSM experts tell us that certain cross sections are not known with the required precision :

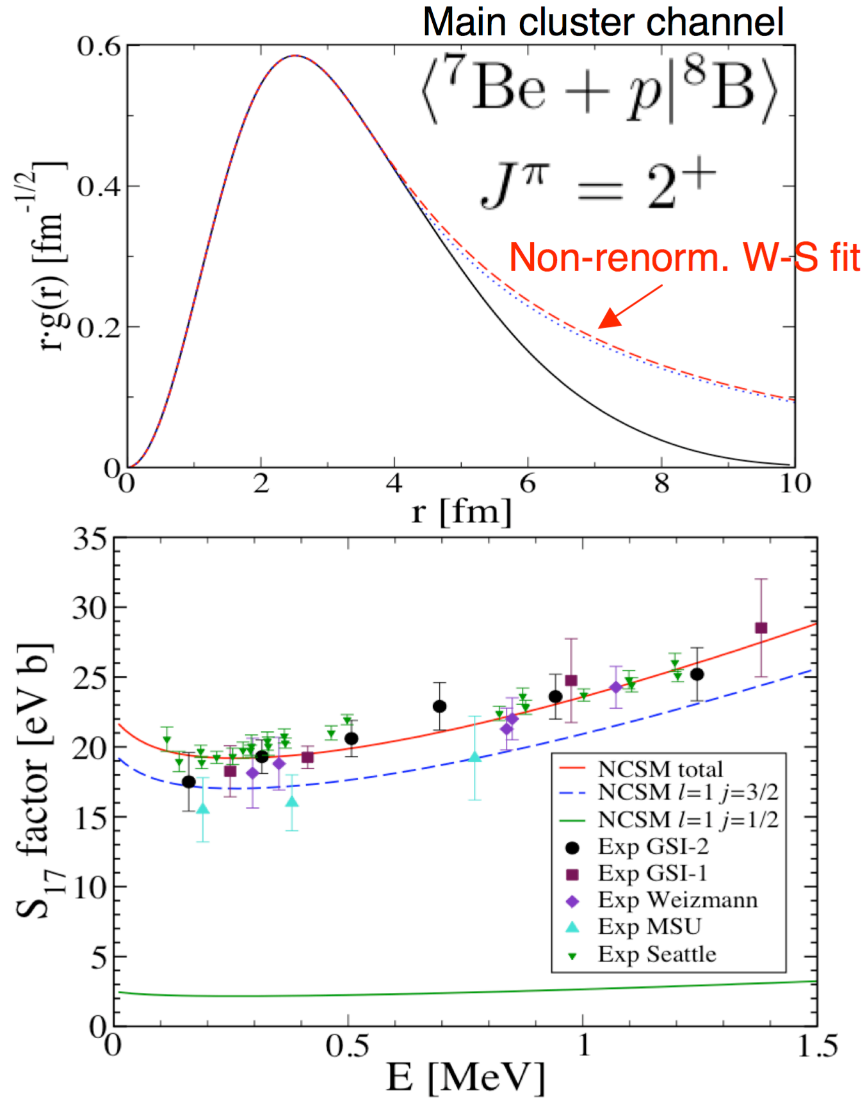
- ^{7}Be(p,γ)^{8}B
- ^{3}He(α,γ)^{7}Be

J.N. Bahcall, PRL 92, 121301 (2004)

^{7}Be(p,γ)^{8}B study

- CD-Bonn 2000 *NN* interaction, model spaces up to 10hΩ
- Cluster overlaps fitted to W-S potential solution in 0-4 fm range
- Scattering state from a potential model that fits ^{8}B(1$^+$) resonance

S_{17} = 22.1 ± 1.0 eV·b



P. Navrátil, et al, Phys. Lett. B 634, 191 (2006)

Results, solar pp chain: $^3He(\alpha,\gamma)^7Be$ - Preliminary!

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- $^7Be(p,\gamma)^8B$
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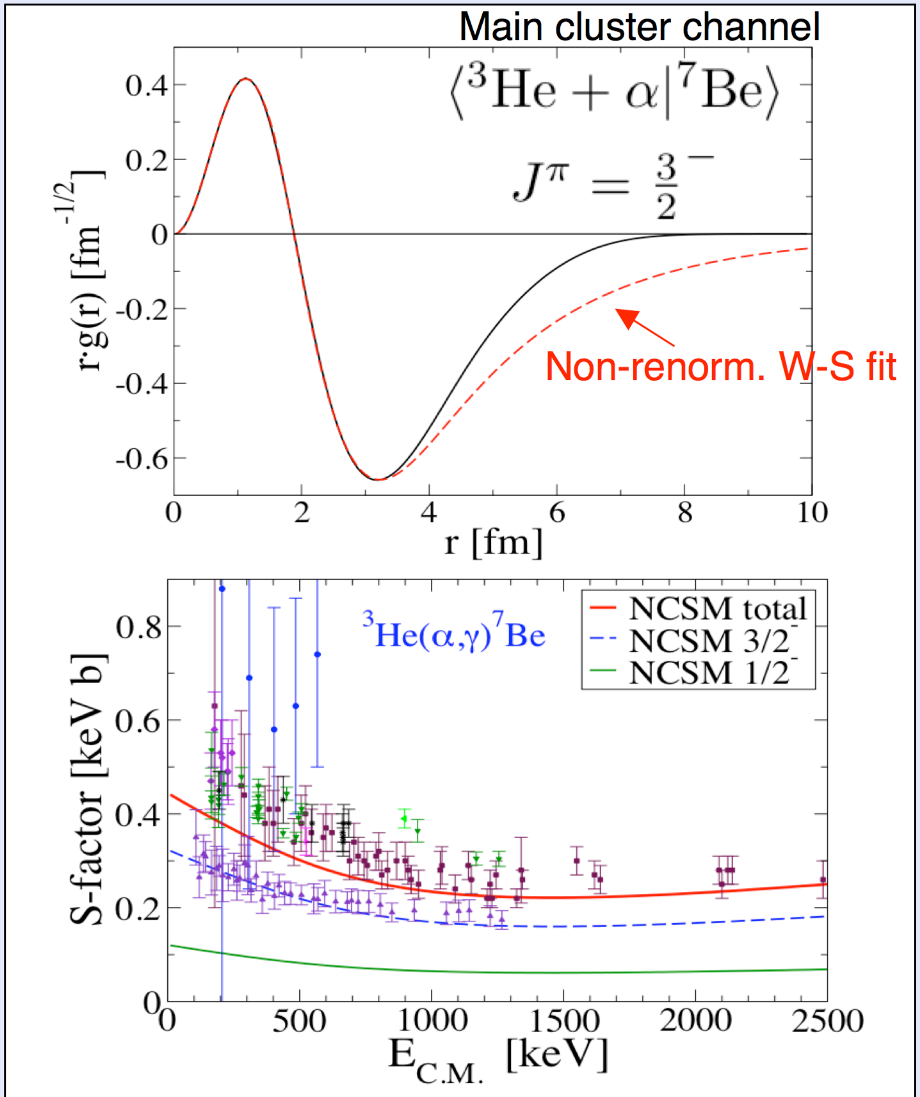
J.N. Bahcall, PRL 92, 121301 (2004)



Preliminary results from P. Navrátil,

$^3He(\alpha,\gamma)^7Be$ study

- CD-Bonn 2000 *NN* interaction, model spaces up to 10hΩ
- Cluster overlaps fitted to W-S potential solution in 0-3.6 fm range
- Scattering state from a potential model that fits phase shifts
- Results similar to K. Nollett's calculations using the VMC overlap

Convergence tests underway…

Summary and outlook

- **We have the tools and techniques to study strongly interacting, fermionic quantum many-body systems.**
- **First attempts of combining *ab initio* nuclear structure information with the modeling of low-energy reactions are being performed.**
- **There are dedicated efforts to achieve a truly fundamental description of nuclear reactions.**

RGM equations, coupled integro-differential equations:

$$\sum_{\nu'} \int d^3r' \left[H_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) - E N_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) \right] \varphi_{\nu'}(\vec{r'}) = 0$$

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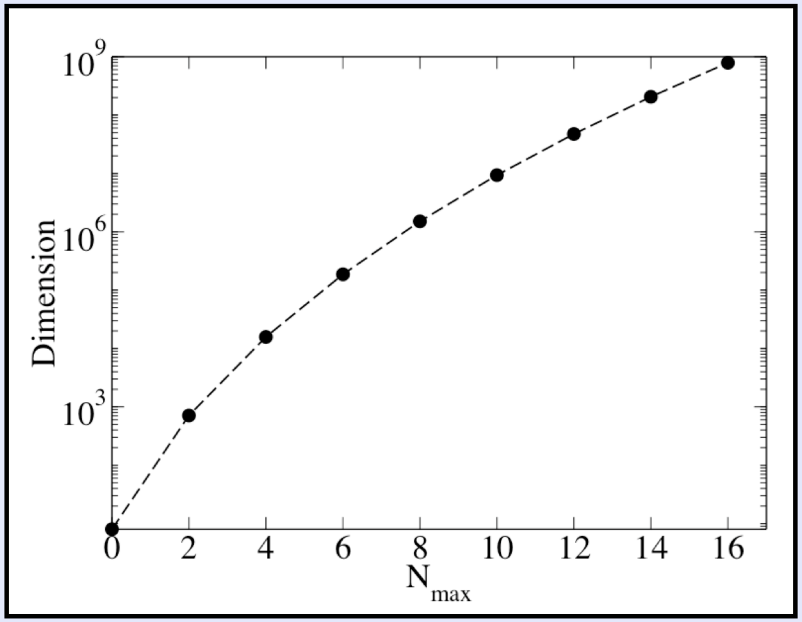
Appendix

Shell model codes and convergence

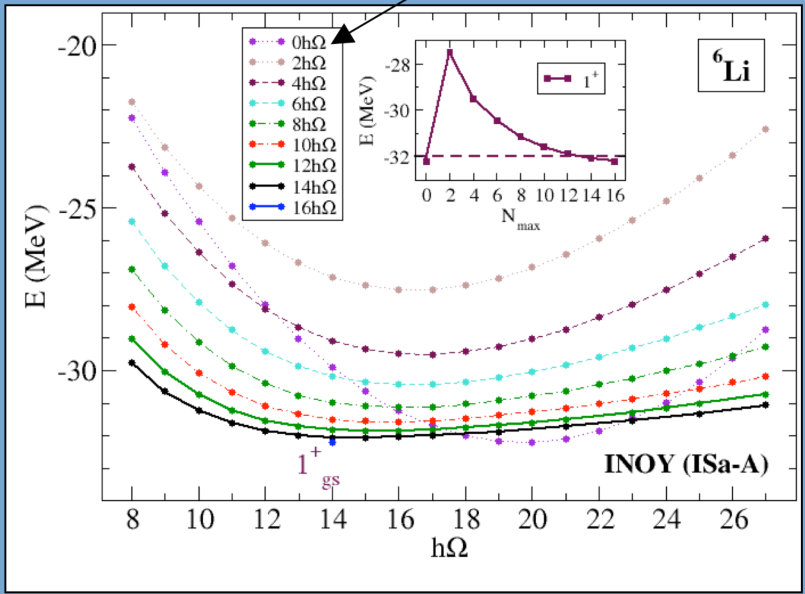
- Diagonalization of huge, but sparse, matrices
- M-scheme shell model codes: MFD, REDSTICK, ANTOINE



^{6}Li(1$^+$) with the INOY interaction:

- Independent of Ω when $N_{max} \rightarrow \infty$
- Not a variational calculation

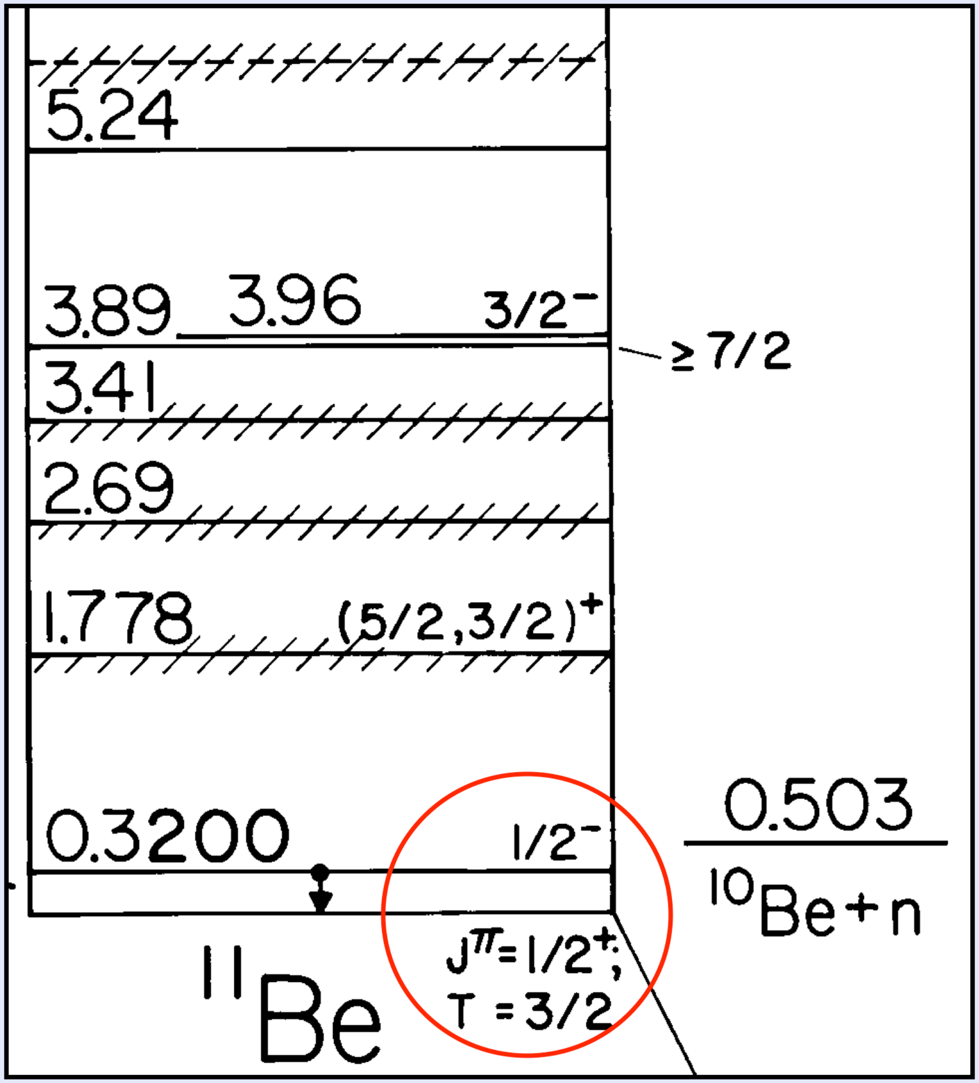
different N_{max}



ANTOINE:

- E. Caurier and F. Nowacki, Acta Phys. Pol. B**30**(1999)705
- Can find eigenvalues of matrices with dimensions ~10^9

A case study: ^{11}Be and its possible role in the early universe

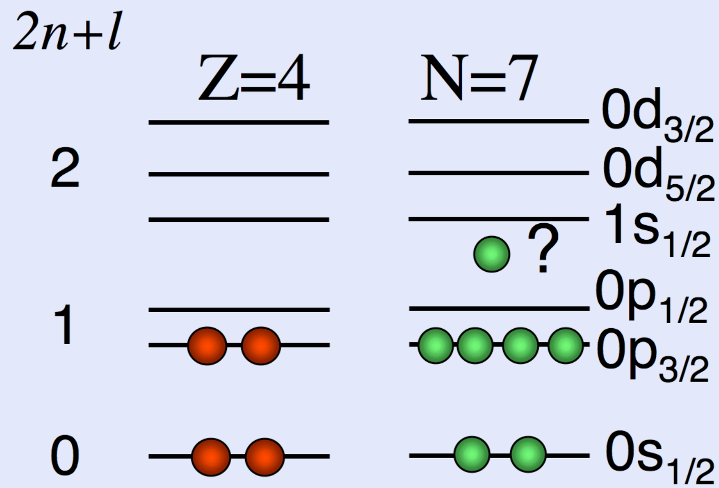


Interesting structure

Quenching of the shell gap

^{11}Be(g.s.) = 1/2$^+$

Talmi and Unna, PRL**4**(1960)469



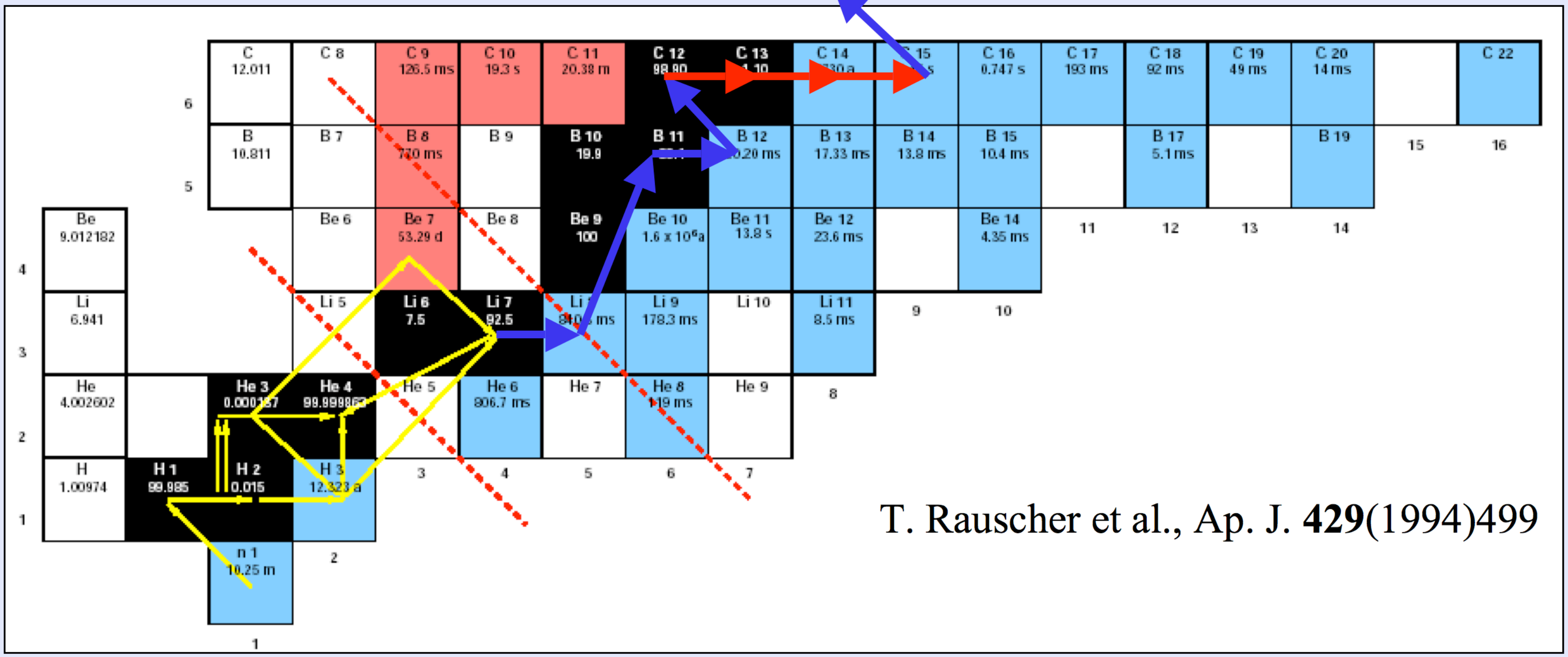
A ^{11}Be 9hΩ model space:

- 66 orbits
- 572 $|nljm\rangle$ s.p. states

^{11}Be in non-standard Big Bang scenarios

Suggestion: Inhomogenities in the distribution of baryons during the primordial nucleosynthesis can lead to the production of heavy elements.

Breakout from the standard Big Bang nucleosynthesis:



T. Rauscher et al., Ap. J. **429**(1994)499

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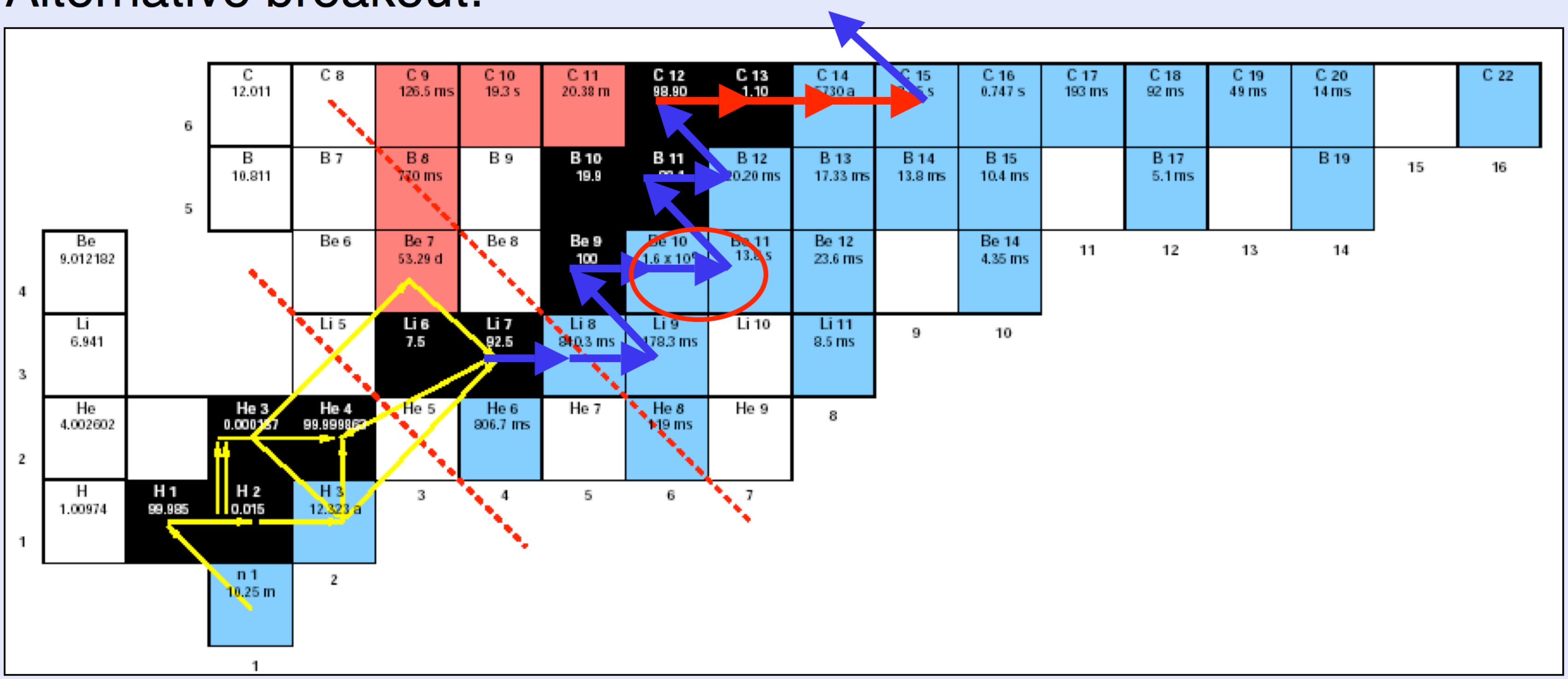
^{11}Be in non-standard Big Bang scenarios

Alternative reaction flows are theoretically possible. Many of the important cross sections have not been measured!

Alternative breakout:



- ^{7}Li(n,γ)^{8}Li(α,n)^{11}B(n,γ)^{12}B(β^{-})^{12}C(n,γ)^{13}C(n,γ)^{14}C(n,γ)^{15}C …
- ^{7}Li(n,γ)^{8}Li(n,γ)^{9}Li(β^{-})^{9}Be(n,γ)^{10}Be(n,γ)^{11}Be(β^{-})^{11}B(n,γ)^{12}B(β^{-})^{12}C(n,γ) …

C. Forssén, NIC-IX, CERN, Geneva, June 29, 2006

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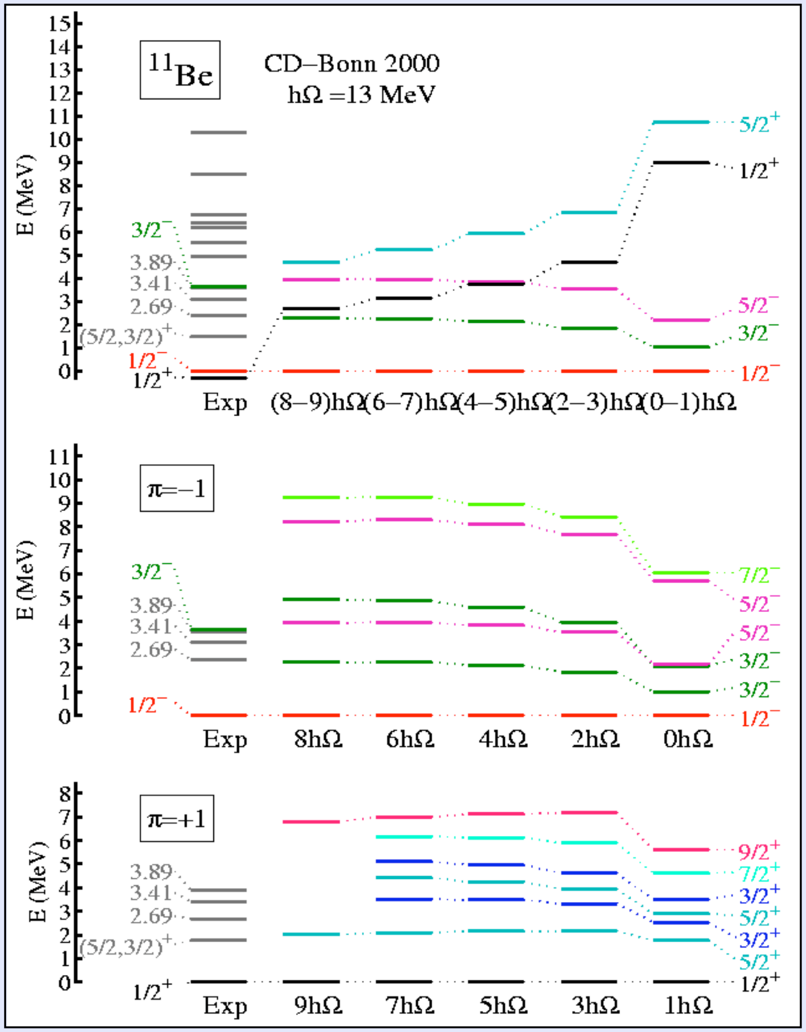
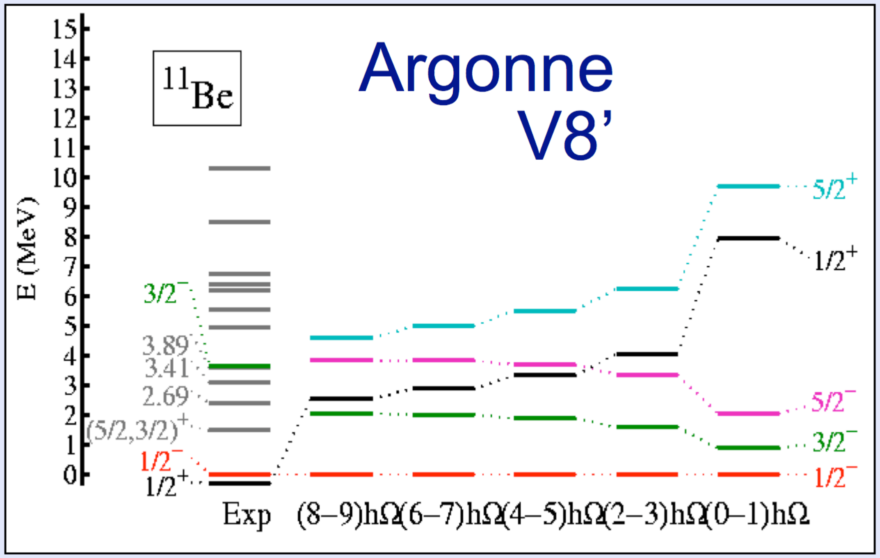
A large-scale *ab initio* NCSM study of $^{9-11}$Be

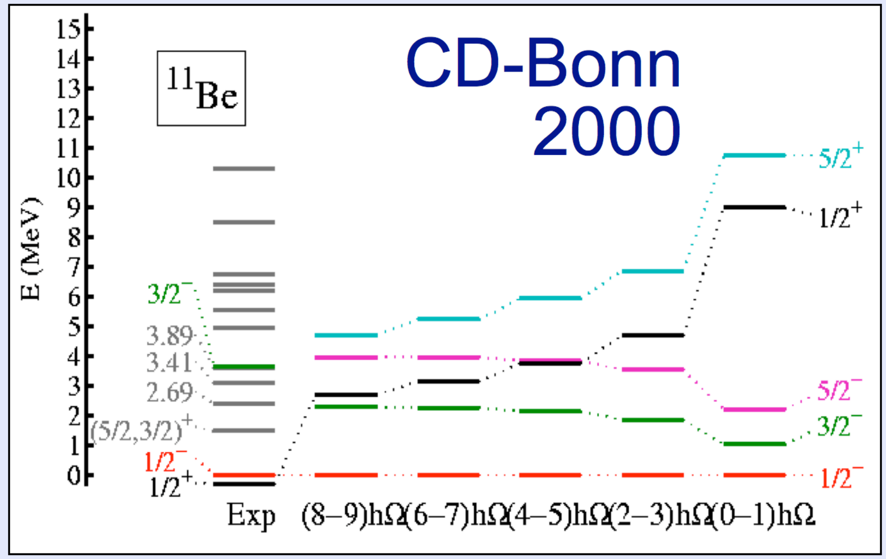
- Large-scale calculations with convergence tests were performed for several A=9-13 isotopes.
- Model spaces exceeding 1×10^9 were reached.
- Effects of different NN interactions on spectroscopy and other observables were studied.
- Particular focus on the parity-inversion, which was not reproduced. Indications that 3N forces are important.
- However, the wave functions seem to be well converged and we can investigate cluster overlaps.

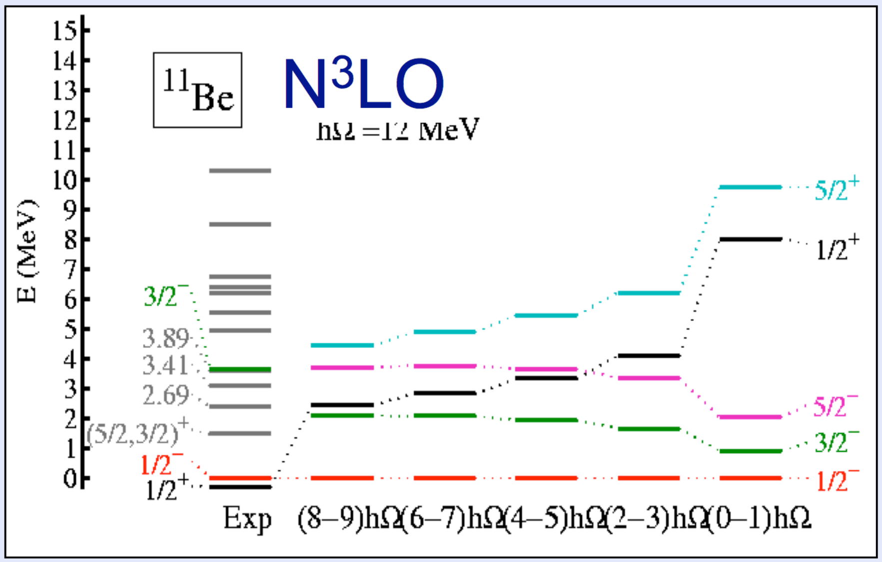


C. Forssén *et al*, Phys. Rev. C 71 (2005) 044312

^{11}Be spectra







- Remarkable agreement between the predictions of different, high-precision *NN* interactions.
- Unnatural-parity states are too high - but dropping.

New possibility: input from *ab initio* nuclear structure

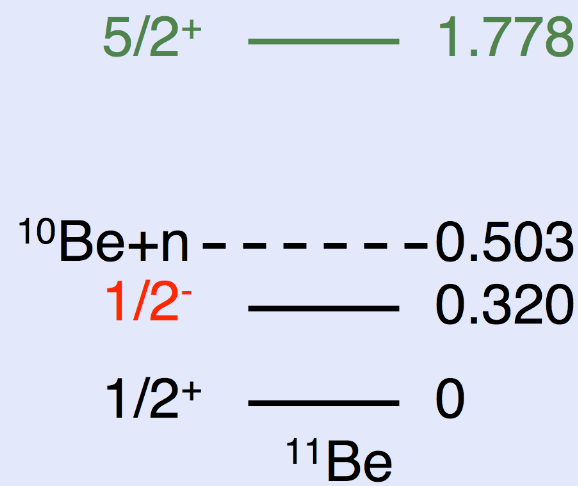
<u>Input from *ab initio* NCSM:</u>

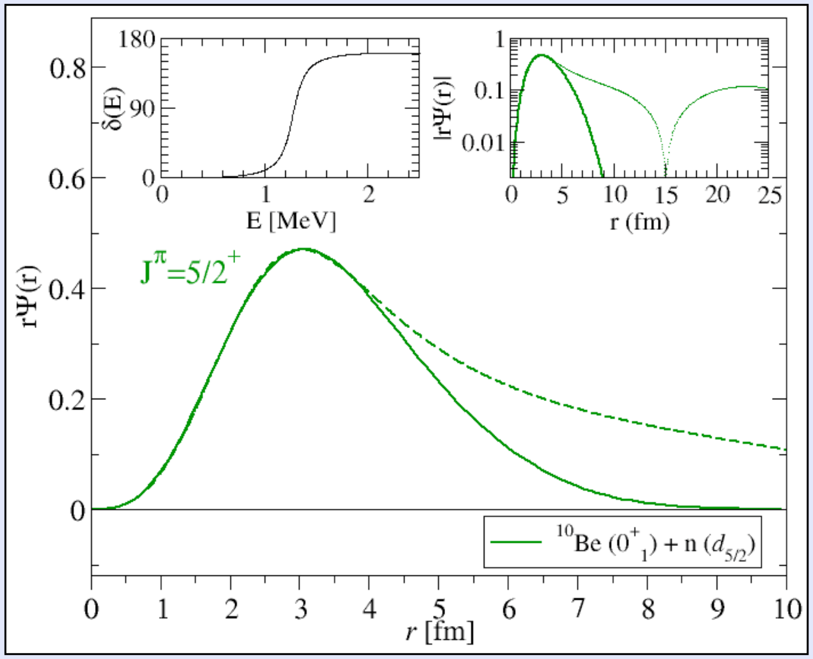
- **Corrected cluster overlaps** with calculated **spectroscopic factors** for the two bound states.

- This procedure also provides **effective interfragment potentials** that are used for *l=0* and *l=1* scattering states.

- An *l=2* effective potential is obtained by a fit to the $^{10}Be_{gs}+n(d_{5/2})$ overlap with the **$5/2^+$ resonance**.

- **E2 transition strength** from the $5/2^+$ resonance obtained from the A-body NCSM calculation

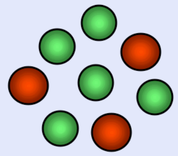




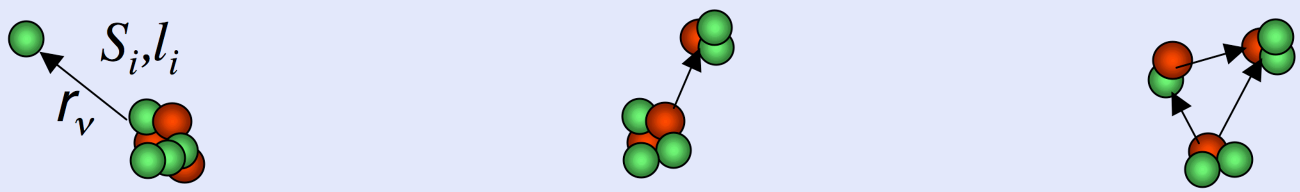
Resonating Group Method - a microscopic approach

$$(H - E)\,\Phi^{(A)} = 0$$

Time-independent Schrödinger equation for A-body scattering.

The A-body system: 

is decomposed into various “channels” ν:



Here, we focus on two-cluster channels:

$$\Phi^{(A)} = \sum_\nu \mathcal{A}_\nu \left\{ \Phi_{1\nu}\Phi_{2\nu}\varphi_\nu(\vec{r}_\nu) \right\} = \sum_\nu \int d^3r\, \varphi_\nu(\vec{r})\Phi_\nu^{(A)}(\vec{r})$$

expansion coefficient

basis functions: $\Phi_\nu^{(A)}(\vec{r}) = \mathcal{A}_\nu \left\{ \Phi_{1\nu}\Phi_{2\nu}\delta\left(\vec{r}_\nu - \vec{r}\right) \right\}$

RGM equations-of-motion

RGM equations, coupled integro-differential equations:

$$\sum_{\nu'} \int d^3r' \left[H_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) - E N_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) \right] \varphi_{\nu'}(\vec{r'}) = 0$$

- The RGM basis functions are non-orthogonal (at short distances):

$$N_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) = \left\langle \Phi_{\nu}^{(A)}(\vec{r}) \middle| \Phi_{\nu'}^{(A)}(\vec{r'}) \right\rangle$$

- *H* is the full, microscopic Hamiltonian (3A-3 coordinates are involved)

$$H_{\nu\nu'}\left(\vec{r}, \vec{r'}\right) = \left\langle \Phi_{\nu}^{(A)}(\vec{r}) \middle| H \middle| \Phi_{\nu'}^{(A)}(\vec{r'}) \right\rangle$$

- A fully orthogonal representation can be found by introducing $N^{1/2}$, $N^{-1/2}$