Determining the underlying probability distributions for the 3α process

James deBoer, University of Notre Dame

Key Reactions in Nuclear Astrophysics (KRINA2025)

Trento, Italy, February 17-21, 2025

IReNA

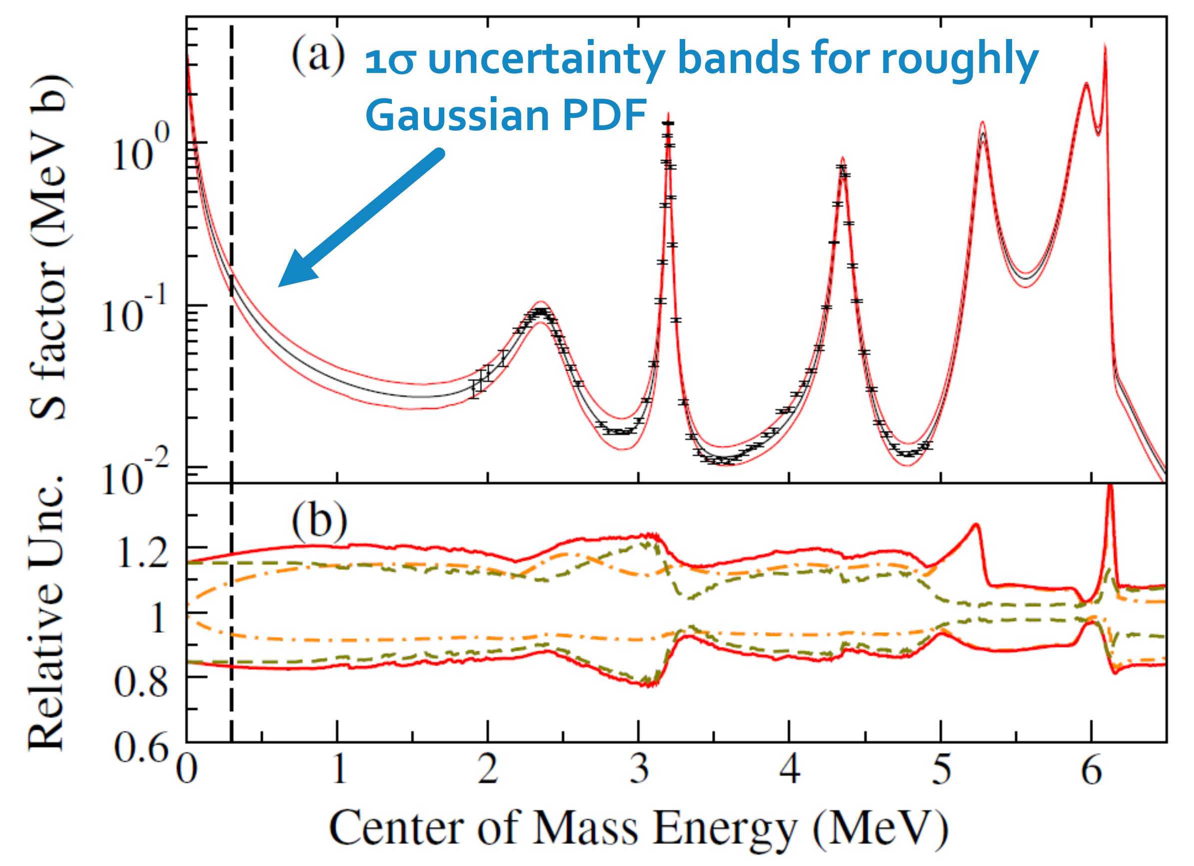
International Research Network for Nuclear Astrophysics

NSF

UNIVERSITY OF NOTRE DAME

This was done for $^{12}C(\alpha,\gamma)^{16}O$, but what about 3α?

- This was the main motivation behind RMP **89**,035007 (2017) article on $^{12}C(\alpha,\gamma)^{16}O$
  - Following Gialanella *et al*. (2001), but with much more data
  - Although there is certainly room for improvement here
  - Roughly Gaussian PDF
  - Very computationally challenging

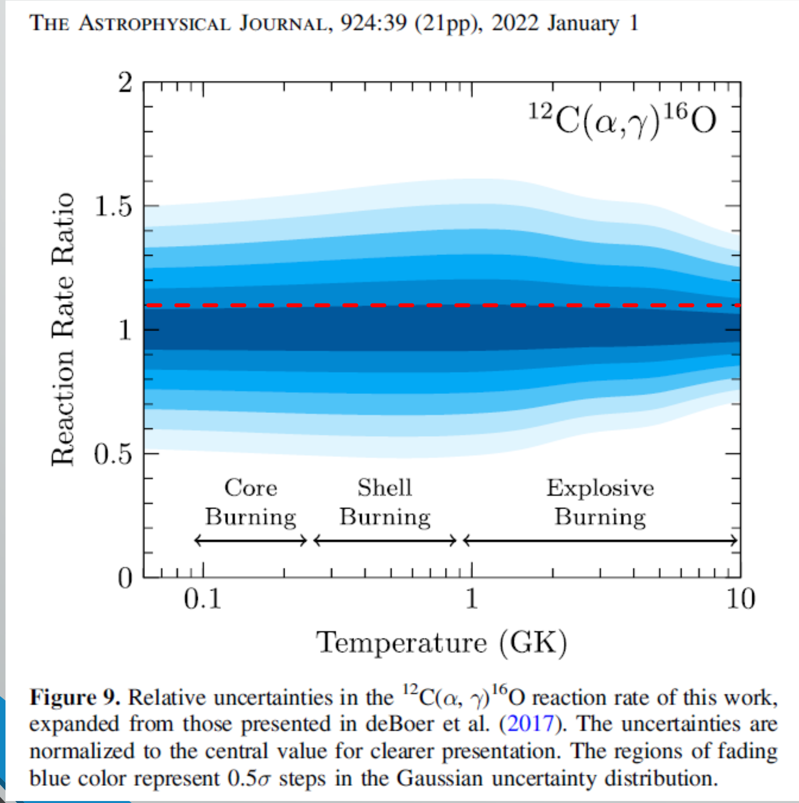


1σ uncertainty bands for roughly Gaussian PDF

Motivation Highlight: Black Hole Mass Gap

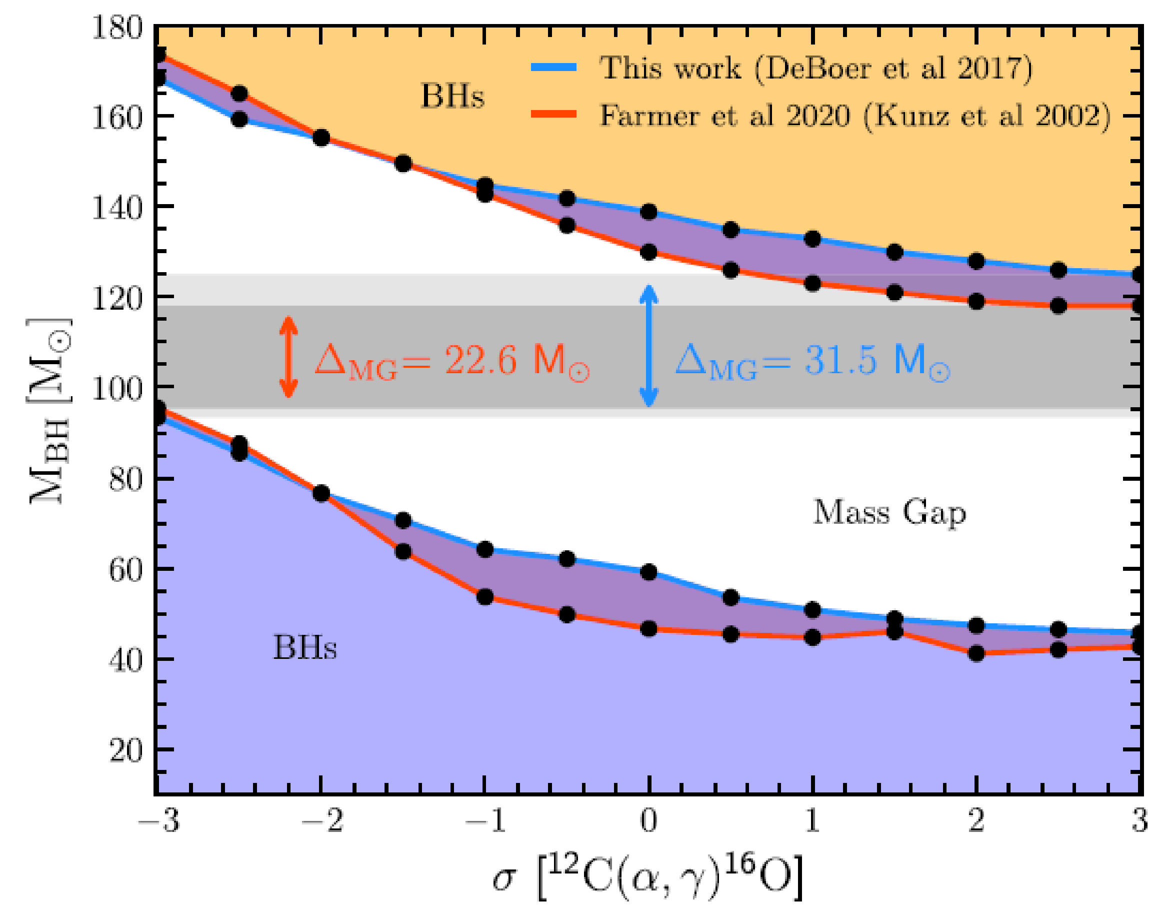
Link to LIGO

- **Farmer *et al.* (2020), Mehta *et al.* (2022)**



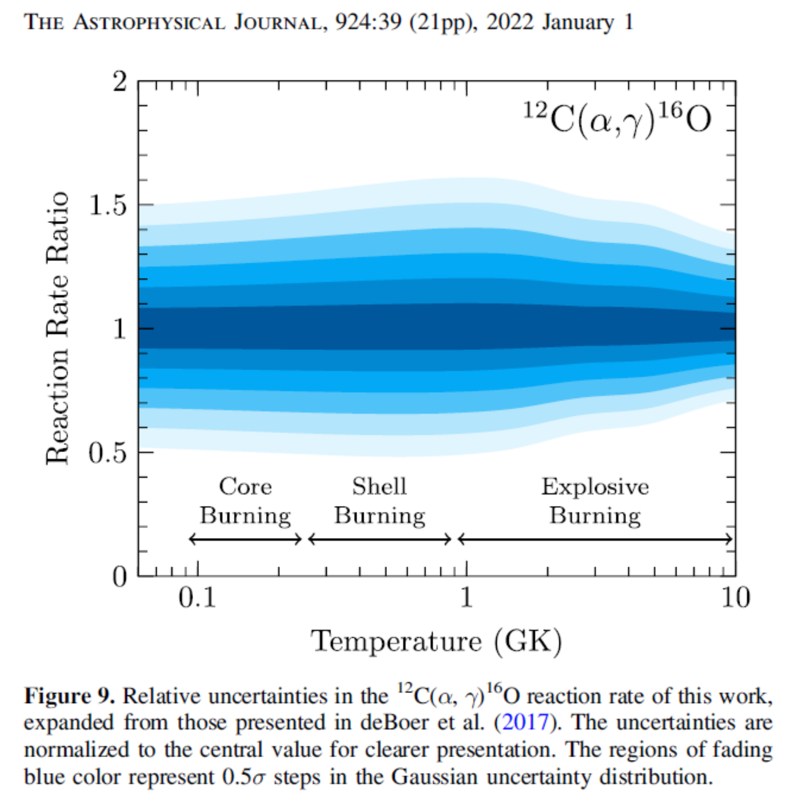
The Astrophysical Journal, 924:39 (21pp), 2022 January 1

Figure 9. Relative uncertainties in the $^{12}C(\alpha,\gamma)^{16}O$ reaction rate of this work, expanded from those presented in deBoer et al. (2017). The uncertainties are normalized to the central value for clearer presentation. The regions of fading blue color represent 0.5σ steps in the Gaussian uncertainty distribution.



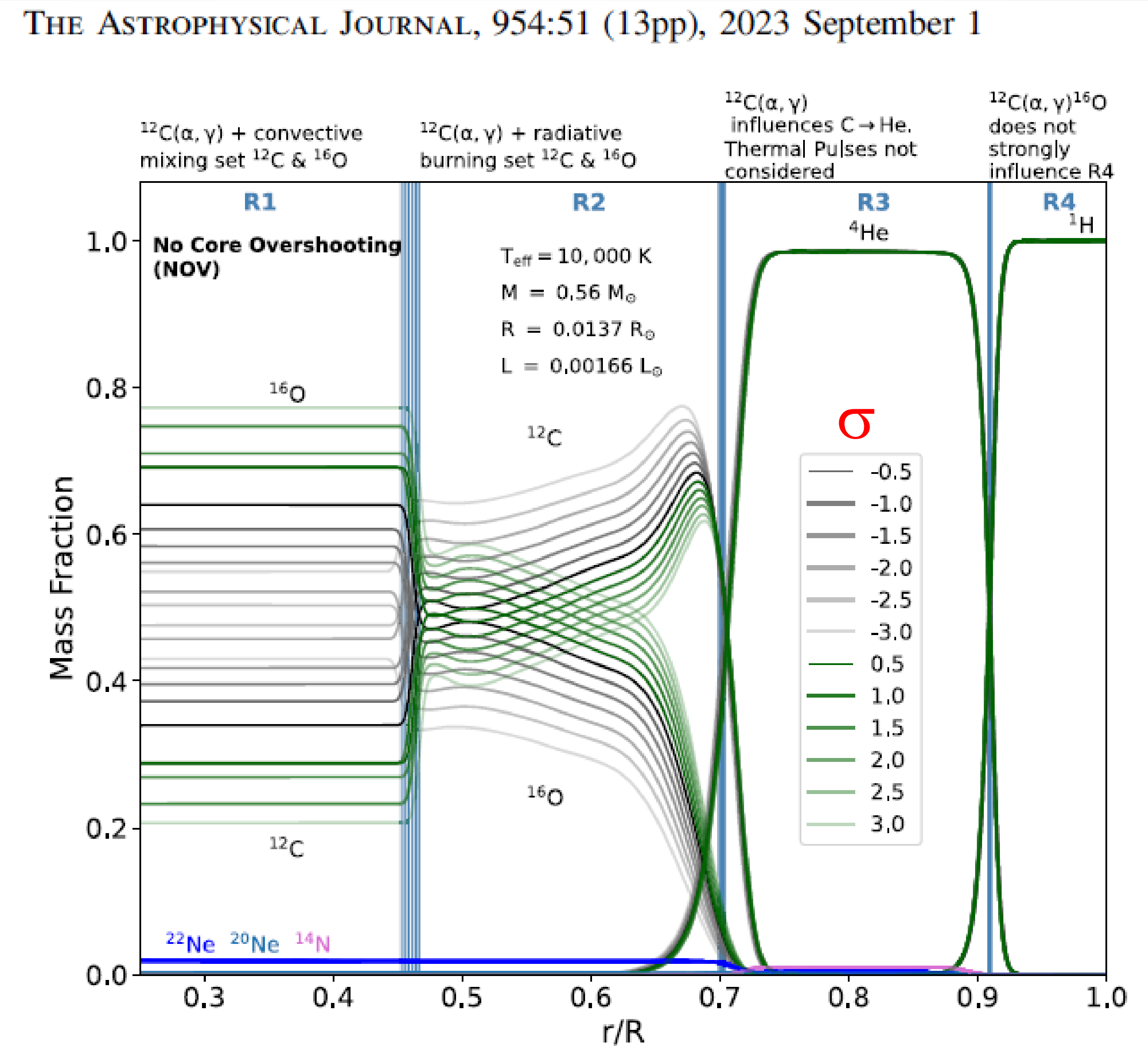
Motivation Highlight: White Dwarf Seismology

- **Chidester *et al*. (2022,2023)**



The Astrophysical Journal, 924:39 (21pp), 2022 January 1

Figure 9. Relative uncertainties in the $^{12}C(\alpha, \gamma)^{16}O$ reaction rate of this work, expanded from those presented in deBoer et al. (2017). The uncertainties are normalized to the central value for clearer presentation. The regions of fading blue color represent 0.5σ steps in the Gaussian uncertainty distribution.



The Astrophysical Journal, 954:51 (13pp), 2023 September 1

Helium burning, a simple process

1. Two helium nuclei fuse to form a very short lived ^{8}Be ground state ($t_{1/2} \approx 0.01$ fs)

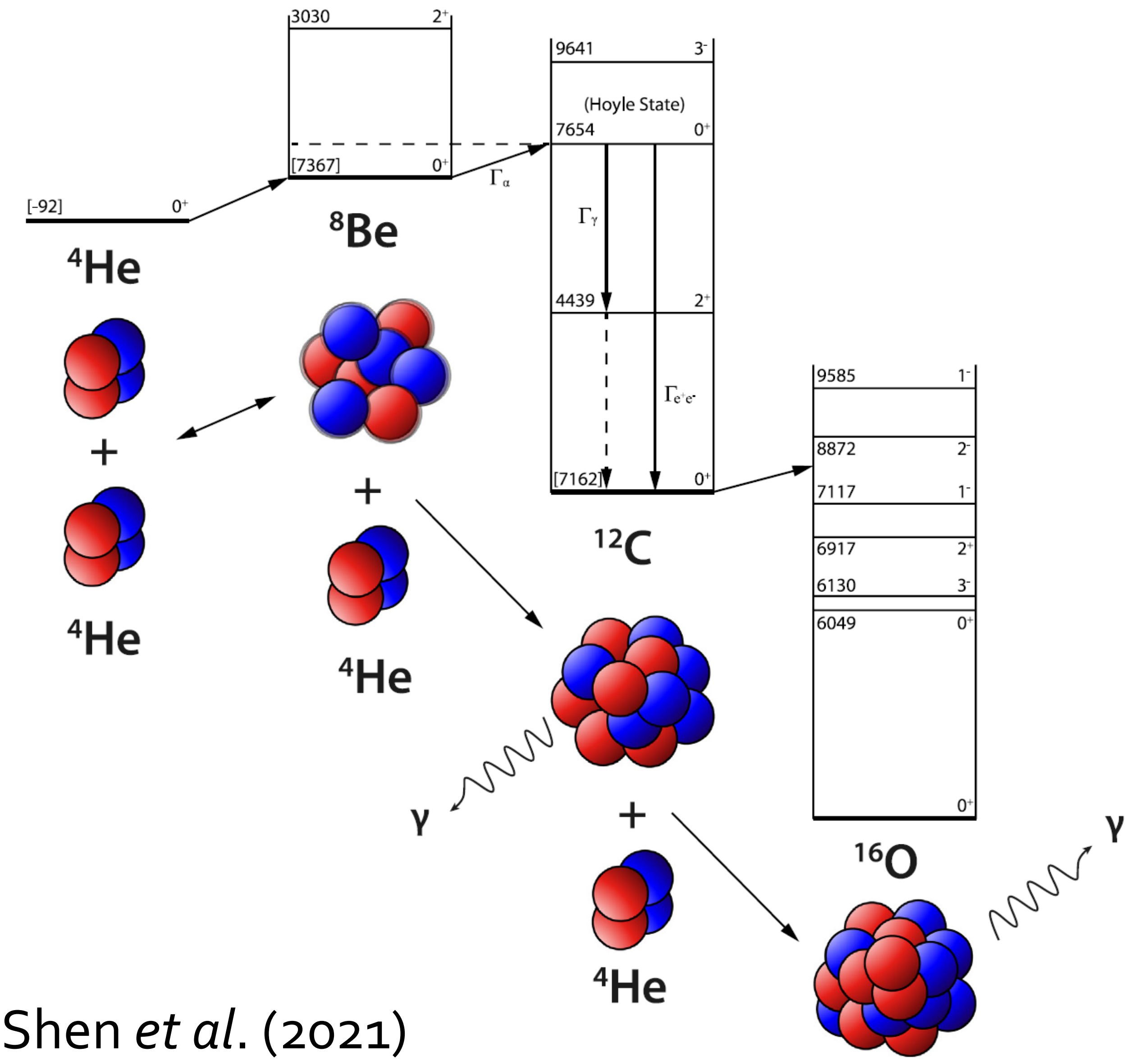
   <αα>

2. A helium nuclei fuses with ^{8}Be to form ^{12}C

   <α^{8}Be>

3. ✓ Stable ^{12}C then fuses with a helium nuclei to form ^{16}O

   <α^{12}C>



Shen *et al.* (2021)

Sequential (2 body)?

$\alpha + \alpha \rightarrow {}^{8}\mathrm{Be} + \alpha \rightarrow {}^{12}\mathrm{C}$

or

Simultaneous (3 body)?

$\alpha + \alpha + \alpha \rightarrow {}^{12}\mathrm{C}$

Sequential (2 body)?

$\alpha+\alpha \rightarrow {}^{8}\mathrm{Be} + \alpha \rightarrow {}^{12}\mathrm{C}$

At normal helium temperatures this mechanism dominates (Hoyle state)

or

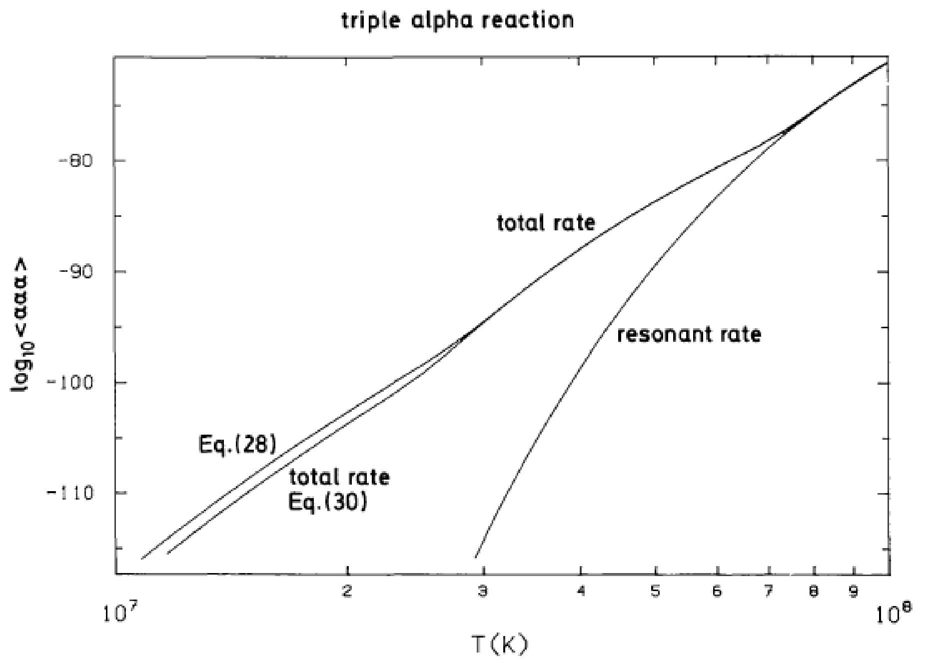
Simultaneous (3 body)?

$\alpha+\alpha+\alpha \rightarrow {}^{12}\mathrm{C}$

At lower temperatures, this may contribute substantially

A brief summary of past calculations

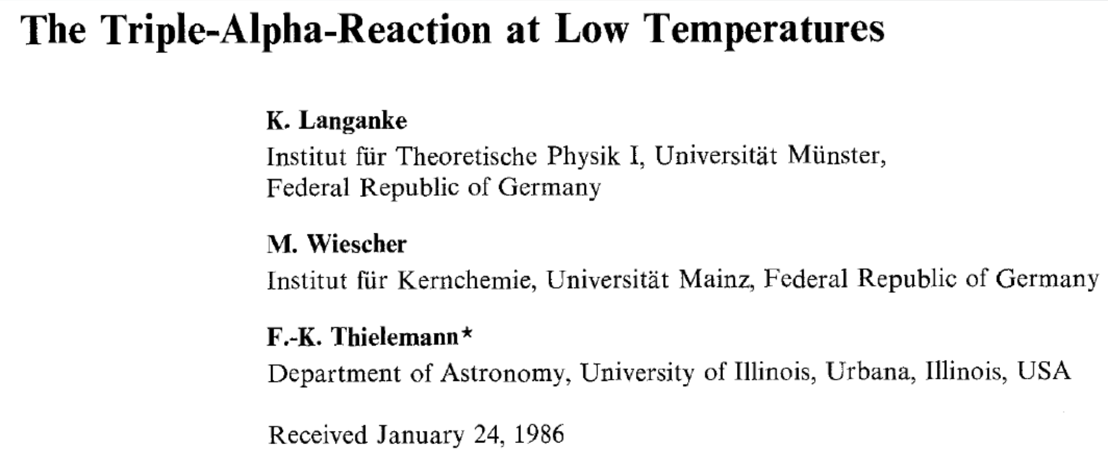
- Still sequential, but with the inclusion of a non-resonant (**direct**) part at low temperatures
    - Nomoto --- ???
    - Langanke --- potential model for $\alpha+\alpha$, direct capture for $^{8}\text{Be}(\alpha,\gamma)^{12}\text{C}$



Astron. Astrophys. 149, 239–245 (1985)

The triple alpha reaction at low temperatures in accreting white dwarfs and neutron stars

K. Nomoto[1,★], **F.-K. Thielemann**[1], **and S. Miyaji**[2]



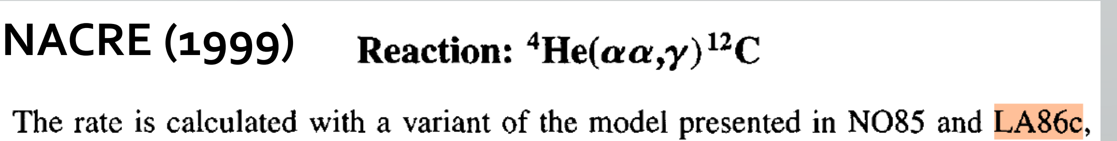
The Triple-Alpha-Reaction at Low Temperatures

K. Langanke
Institut für Theoretische Physik I, Universität Münster,
Federal Republic of Germany

M. Wiescher
Institut für Kernchemie, Universität Mainz, Federal Republic of Germany

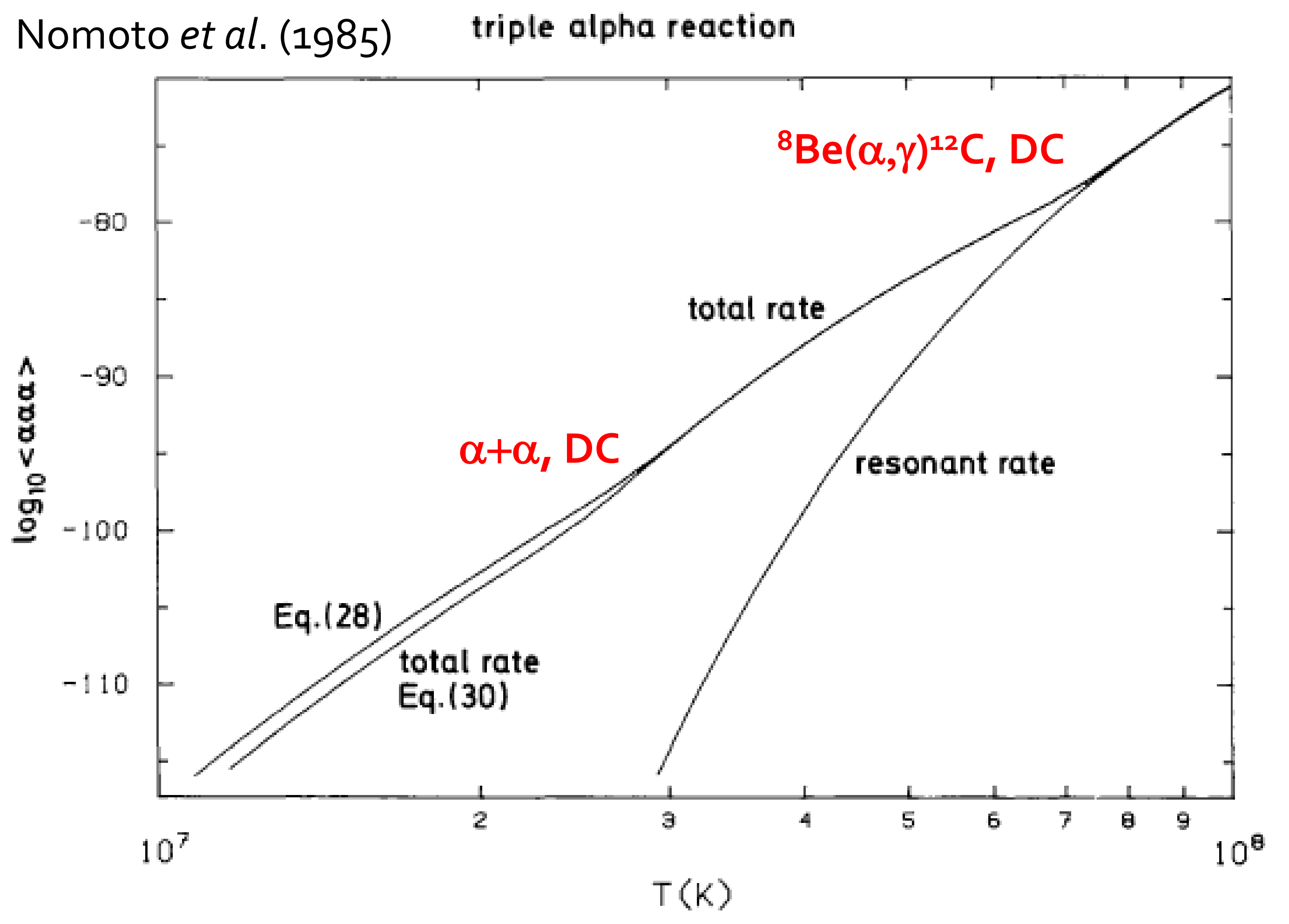
F.-K. Thielemann★
Department of Astronomy, University of Illinois, Urbana, Illinois, USA

Received January 24, 1986



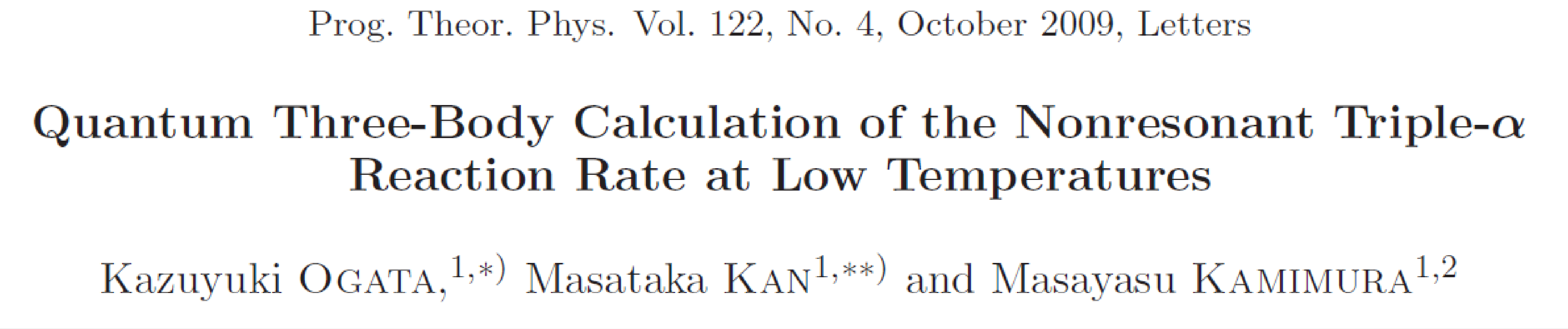
NACRE (1999) **Reaction: $^{4}\text{He}(\alpha\alpha,\gamma)^{12}\text{C}$**

The rate is calculated with a variant of the model presented in NO85 and LA86c,



Nomoto *et al*. (1985)

Fig. 4. The triple-α reaction rate in the temperature range 10^7 K $< T < 10^8$ K. At high temperatures, the resonant rate and the present prediction coincide. Two kinks can be observed at 7.4 10^7 K and 2.8 10^7 K, where the rates for $^{8}\mathrm{Be}(\alpha,\gamma)^{12}\mathrm{C}$ and $\alpha+\alpha \rightleftarrows {}^{8}\mathrm{Be}$ become nonresonant, respectively. In the nonresonant regime of the $\alpha+\alpha$ reaction, the total rate given by Eq. (30) is smaller than that by Eq. (28) because ^{8}Be is produced below the resonance energy at 91.78 keV (see also Fig. 3)

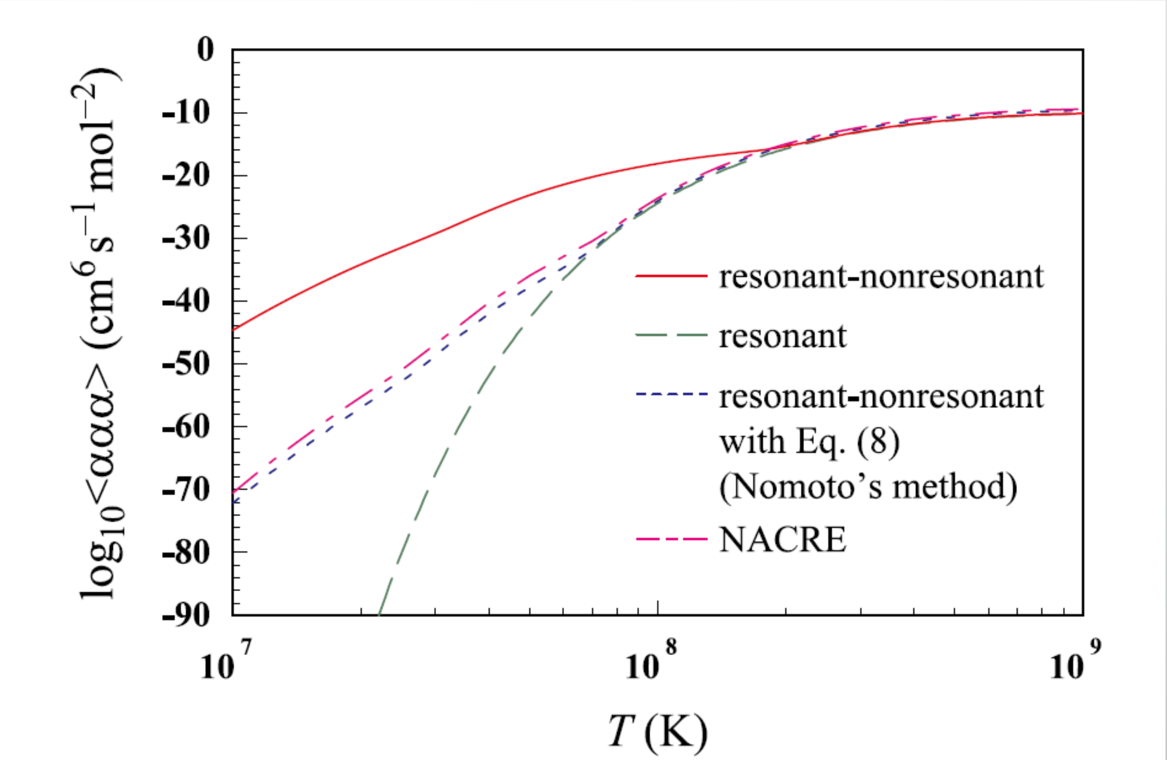


Prog. Theor. Phys. Vol. 122, No. 4, October 2009, Letters

Quantum Three-Body Calculation of the Nonresonant Triple-α Reaction Rate at Low Temperatures

Kazuyuki Ogata,[1,*)] Masataka Kan[1,**)] and Masayasu Kamimura[1,2]

- First 3 body calculations?
- Extremely large low temperature enhancement!
- Seems to be incorrect, but it brought attention to the topic



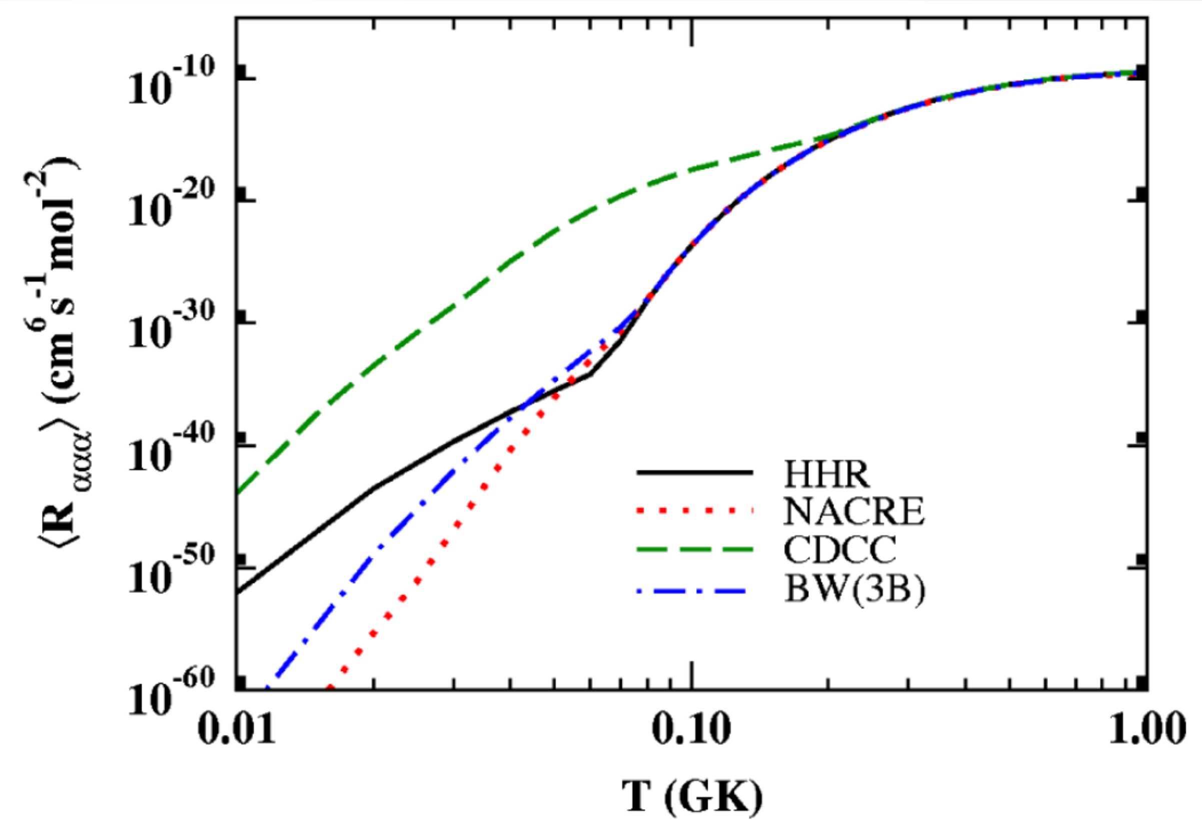
State of the art for the 3α rate

PRL 109, 141101 (2012) PHYSICAL REVIEW LETTERS week ending 5 OCTOBER 2012

Low-Temperature Triple-Alpha Rate in a Full Three-Body Nuclear Model

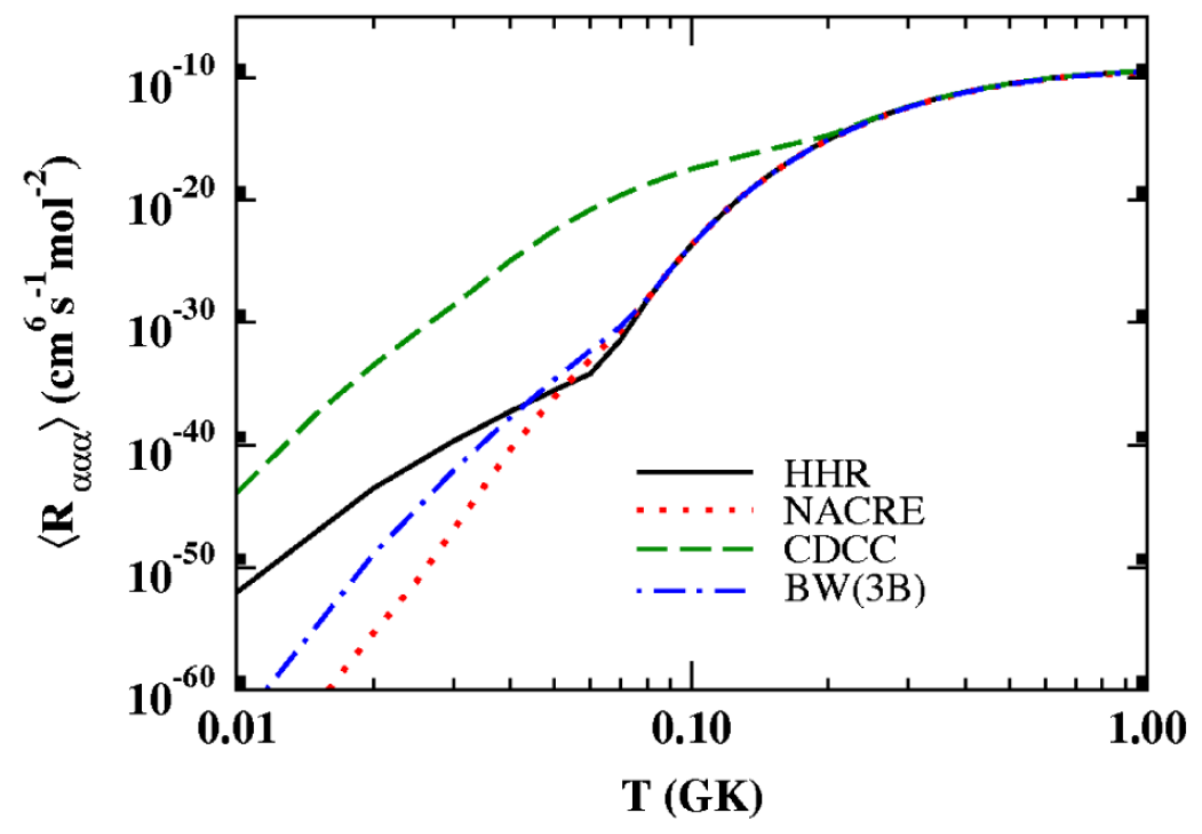
N. B. Nguyen,[1,*] F. M. Nunes,[1,†] I. J. Thompson,[2] and E. F. Brown[1,3]

- Nguyen, Nunes, Thompson and Brown, PRL 109 141101 (2012) and Nguyen, Nunes and Thompson PRC 87, 054615 (2013)
- Hyperspherical Harmonic R-matrix (HHR) --- calculable R-matrix
- Continuum Discretized Coupled Channels (CDCC) --- problem with dealing with scattering of charged particles
- 3 body Breit-Wigner, BW(3B) --- Numerical issues with the calculations
- NACRE --- Purely sequential approximation



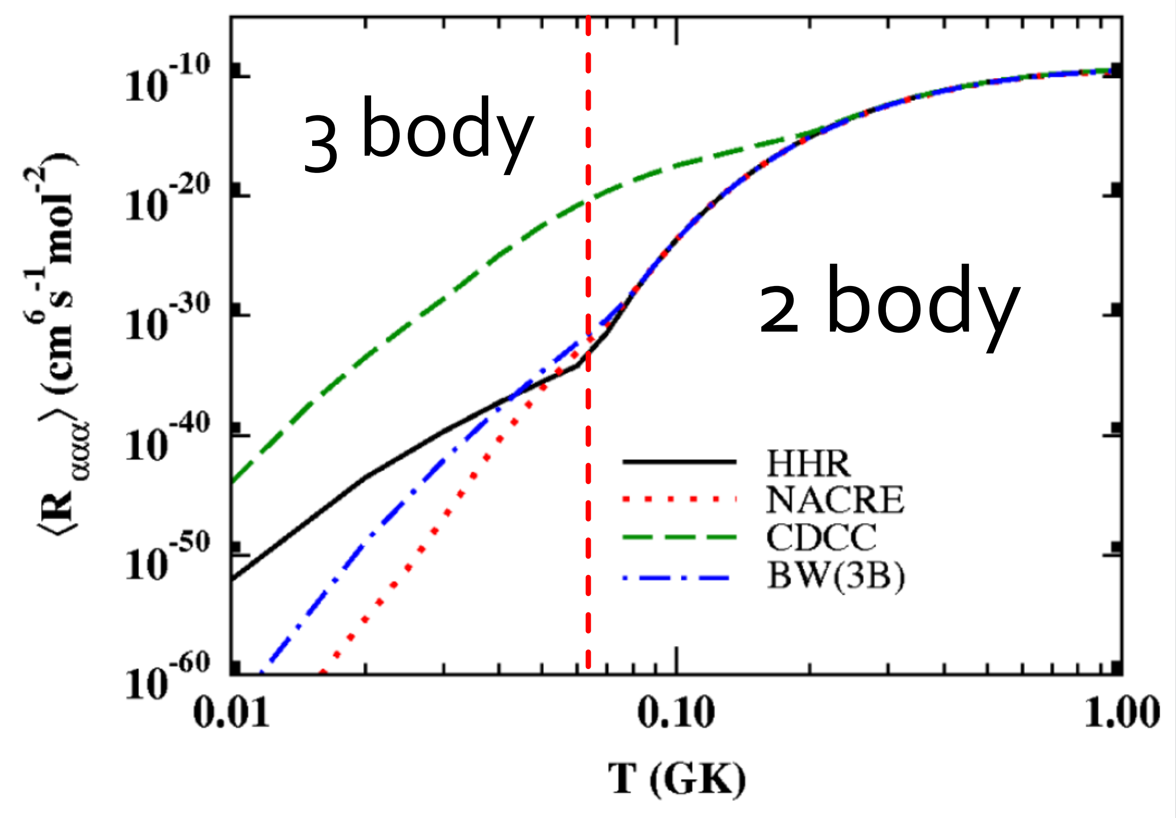
But how important is the simultaneous channel really?

- This diagram makes it look like it is quite important, but how the direct part, maybe even the 2 body part, of the cross section could be calculated very differently
- It would be very useful to see these calculations decomposed into their 2 and 3 body contributions



Uncertainty estimation strategies

- Propagate model uncertainties through the full 3 body formalism
  - Probably can't be done because of long computation times and accessibility?
- Part 2 body, party 3 body
  - Calculate some more limited sensitivity study of the 3 body direct part using the full model to give something like upper and lower limits for the low temperature region
  - Calculate the higher temperature region using usual 2 body formalism



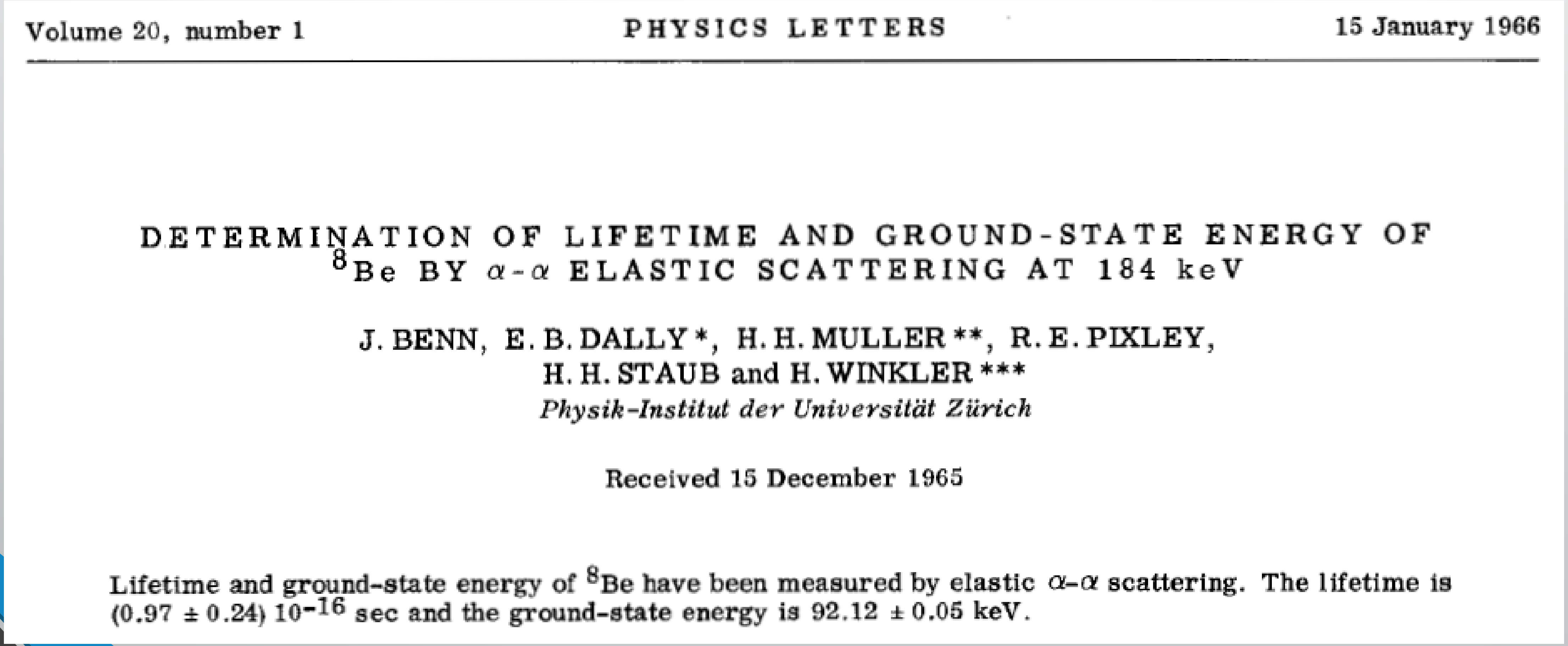
Where can some R-matrix fits and calculations be useful?

- $^{12}C(\alpha,\gamma)^{16}O$
  - Cross section is the result of broad resonances and subthreshold states
  - We can at least measure the energy dependence of the cross section directly
  - Current data gives a pretty good constraint on the interference between resonances
  - Two body type reaction dominates at all energies

- 3α
  - $\alpha+\alpha$ and $^{8}Be(\alpha,\gamma)^{12}C$ are often dominated by narrow resonances
  - We can only measure the level properties of the Hoyle state, but we can do this very well
  - No information on how the Hoyle state interferes with direct part of the cross section
  - Some higher energy $^{12}C(\gamma,\alpha)\alpha$ data
  - 3 body reaction plays a role off resonance

<αα>

- Surprisingly, not very many direct measurements!
- Classic measurement, $\Gamma_{c.m.}$ = 6.8(17) eV, $E_{R,c.m.}$ = 92.12(5) keV



Volume 20, number 1 PHYSICS LETTERS 15 January 1966

DETERMINATION OF LIFETIME AND GROUND-STATE ENERGY OF ^{8}Be BY α-α ELASTIC SCATTERING AT 184 keV

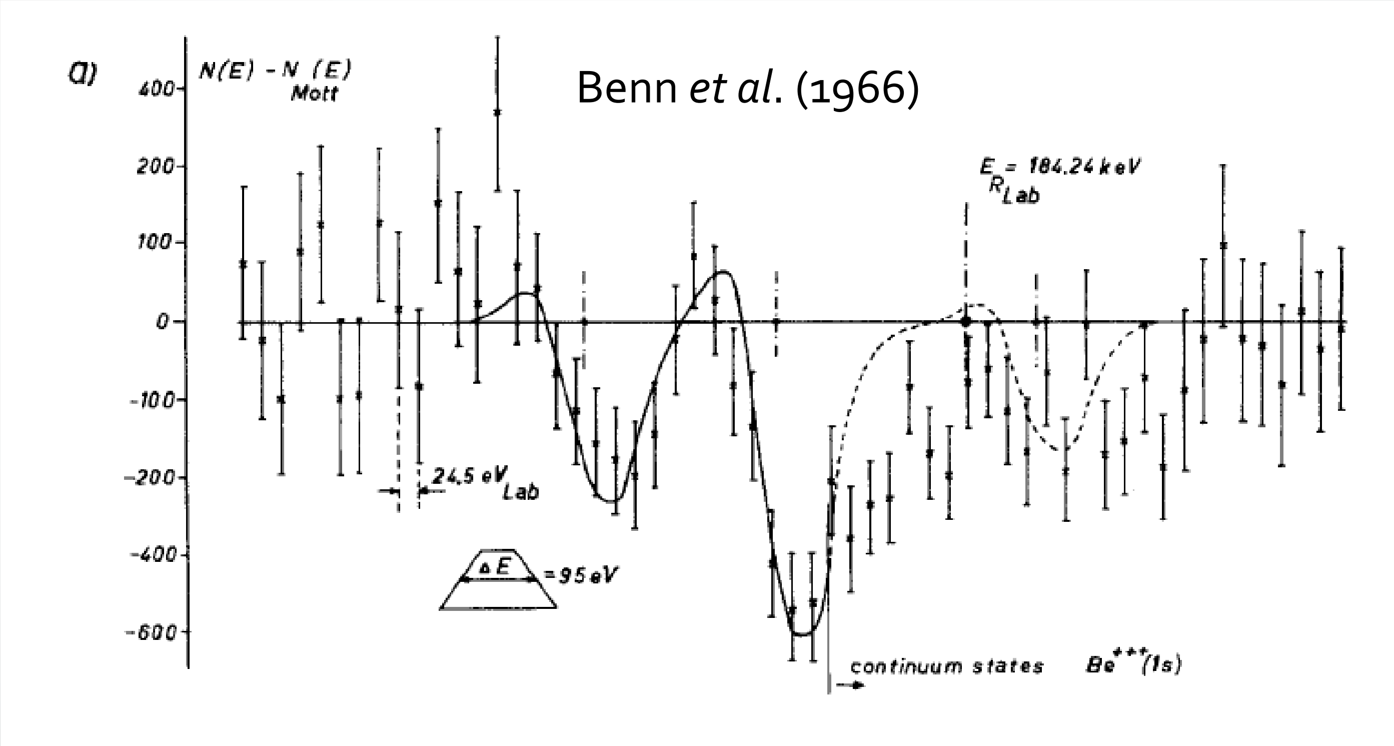
J. BENN, E. B. DALLY *, H. H. MULLER **, R. E. PIXLEY,
H. H. STAUB and H. WINKLER ***
Physik-Institut der Universität Zürich

Received 15 December 1965

Lifetime and ground-state energy of ^{8}Be have been measured by elastic α–α scattering. The lifetime is (0.97 ± 0.24) 10^{-16} sec and the ground-state energy is 92.12 ± 0.05 keV.

<αα>

- **More complicated than one might think**
- One would naïvely expect one peak for the nuclear resonance
- Three peak structure is attributed to the effects of orbital electrons



Benn *et al*. (1966)

<αα>

- Really only one other measurement

Atomic effects on α–α scattering to the ^{8}Be ground state

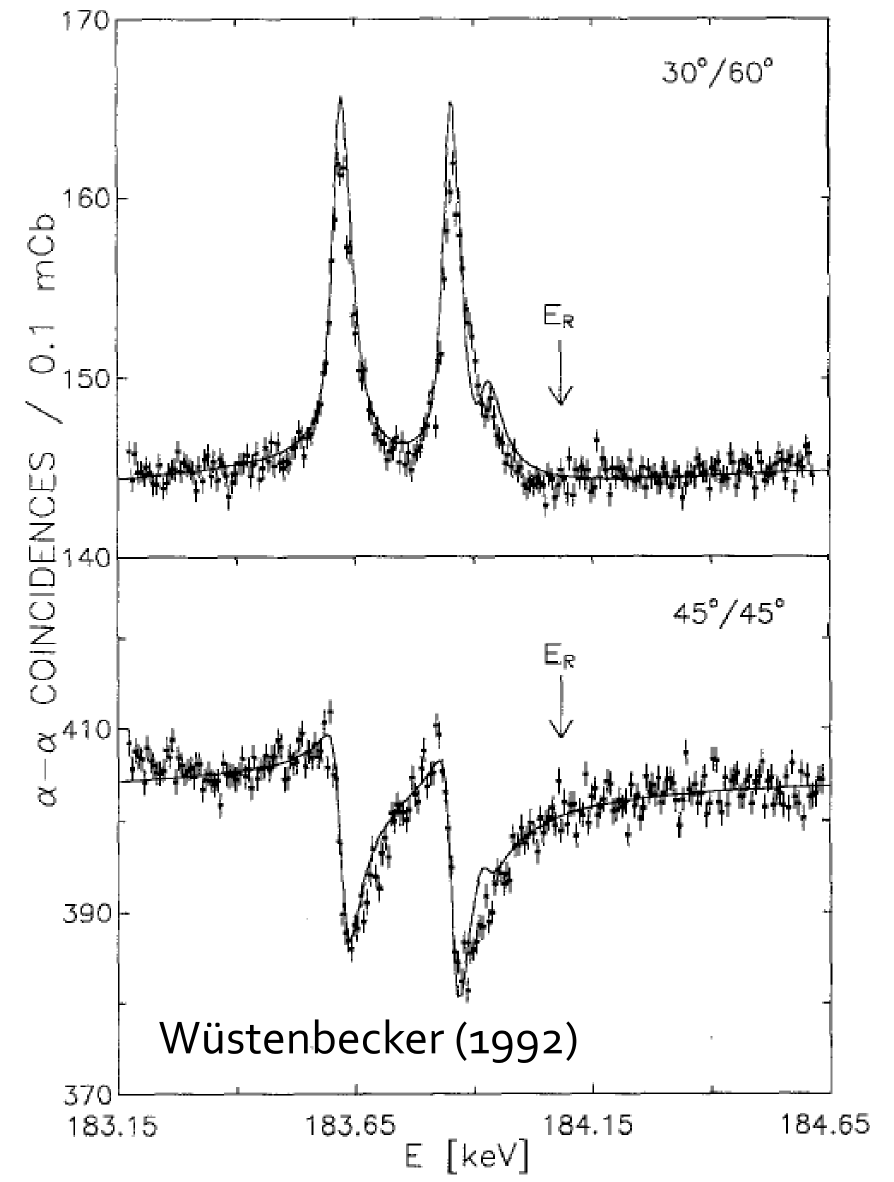
S. Wüstenbecker[1], H.W. Becker[1], H. Ebbing[1], W.H. Schulte[1], M. Berheide[2], M. Buschmann[2], C. Rolfs[2], G.E. Mitchell[3], J.S. Schweitzer[4]

[1] Institut für Kernphysik, Universität Münster, Wilhelm-Klemm-Strasse 4, W-4400 Münster, Federal Republic of Germany
[2] Institut für Experimentalphysik III, Ruhr-Universität Bochum, Postfach 102148, W-4630 Bochum, Federal Republic of Germany
[3] North Carolina State University, Raleigh, NC, USA, and Triangle Universities Nuclear Laboratory, Durham, NC, USA
[4] Schlumberger-Doll Research, Ridgefield, CT, USA

Received: 1 June 1992

<αα>

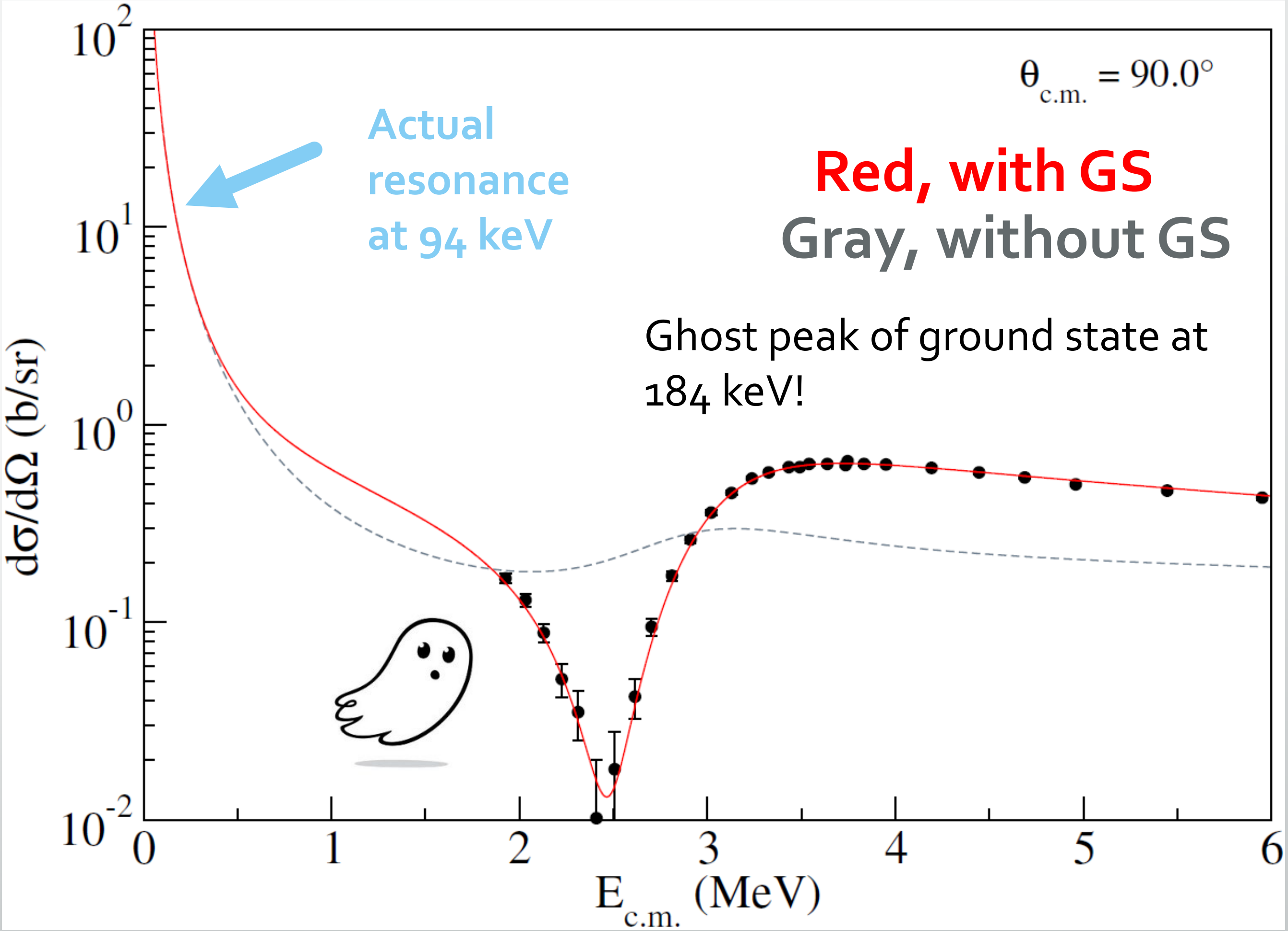
- Much high resolution and statistics than Benn *et al*. (1966)
- Uncertainties due to atomic effects dominate and are harder to quantify
- $\Gamma_{c.m.}$= 5.57(25) eV, $E_{R,c.m.}$ = 92.04(7) keV



Wüstenbecker (1992)

<αα>

- An alternative approach obtaining the width, higher energy αα scattering (fit “ghost” peak)
- Lends itself well to a phenomenological R-matrix analysis
- Only two data sets
  - Haydenburg and Temmer (1956)
  - Tombrello and Senhouse (1963)



Actual resonance at 94 keV

Red, with GS

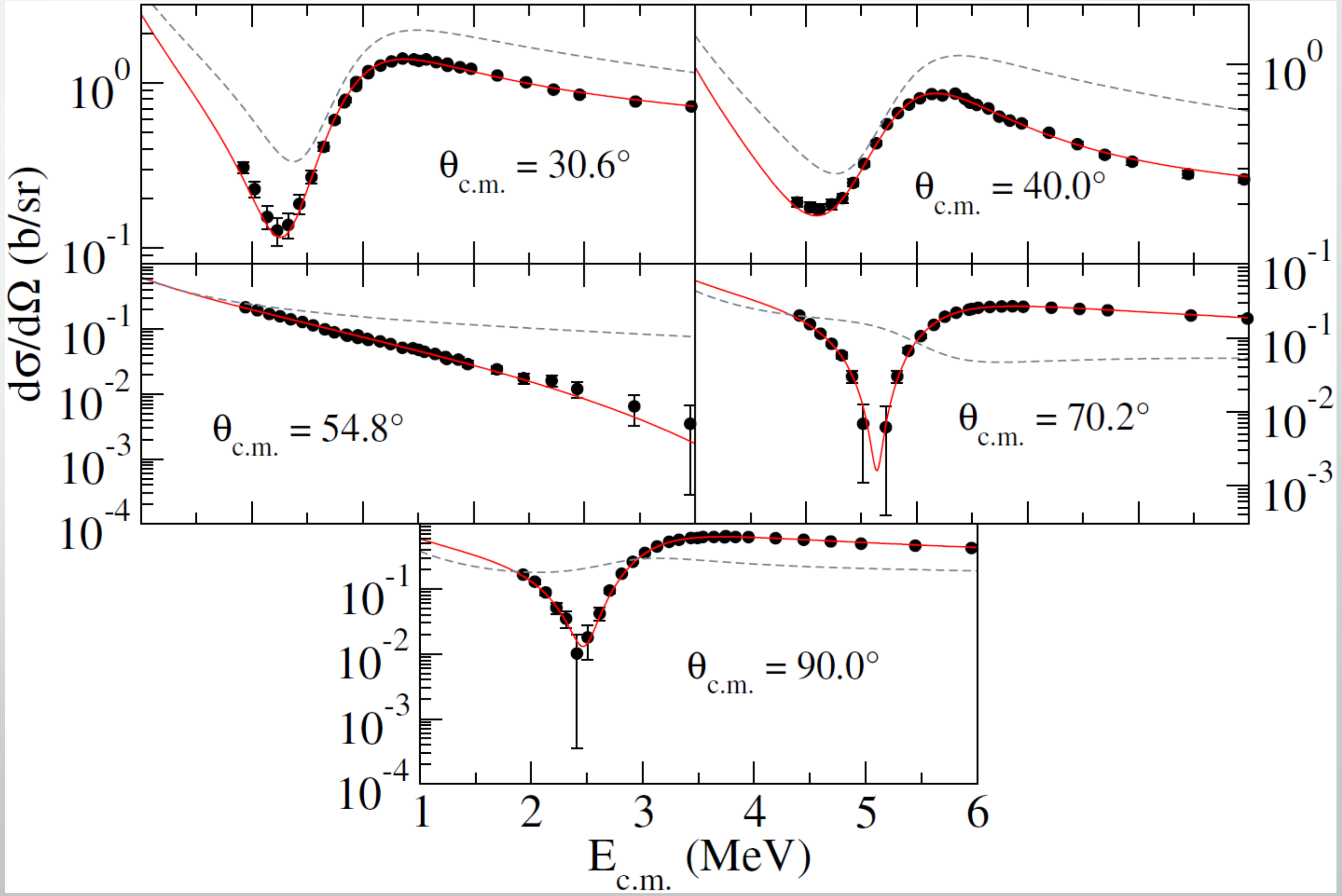
Gray, without GS

Ghost peak of ground state at 184 keV!

<αα>

Fit to αα scattering differential cross section data directly

- Tombrello and Senhouse (1963)
- Quite a good description of the experimental data
- R-matrix code AZURE2



What is BRICK?

- BRICK is a Python package that serves as an interface to AZURE2 and readily permits the MCMC sampling of R-matrix parameters.
  - https://pypi.org/project/brick-james/
- Written by Daniel Odell while a postdoc at Ohio University with Daniel Phillips
  - https://bandframework.github.io/

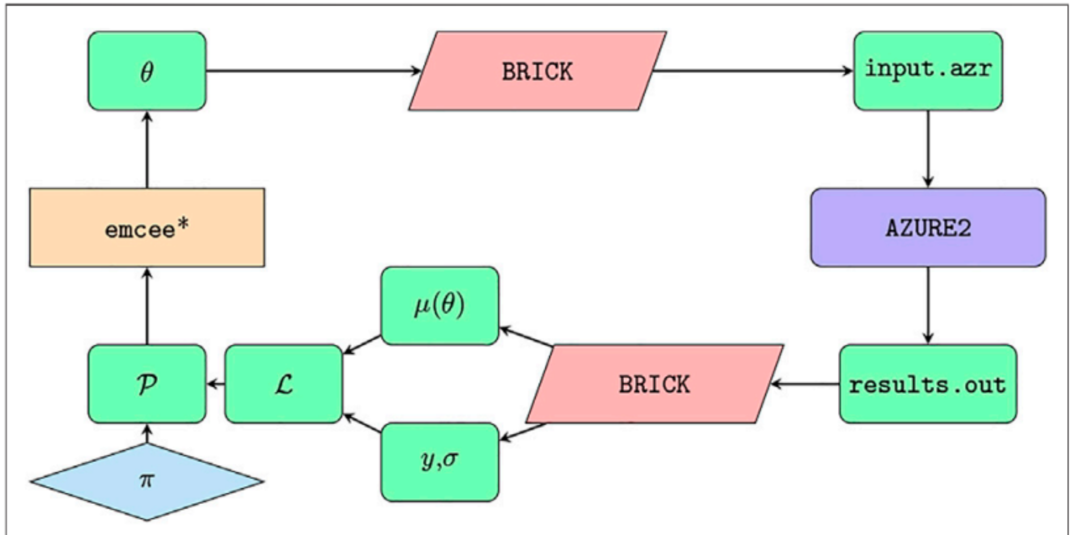
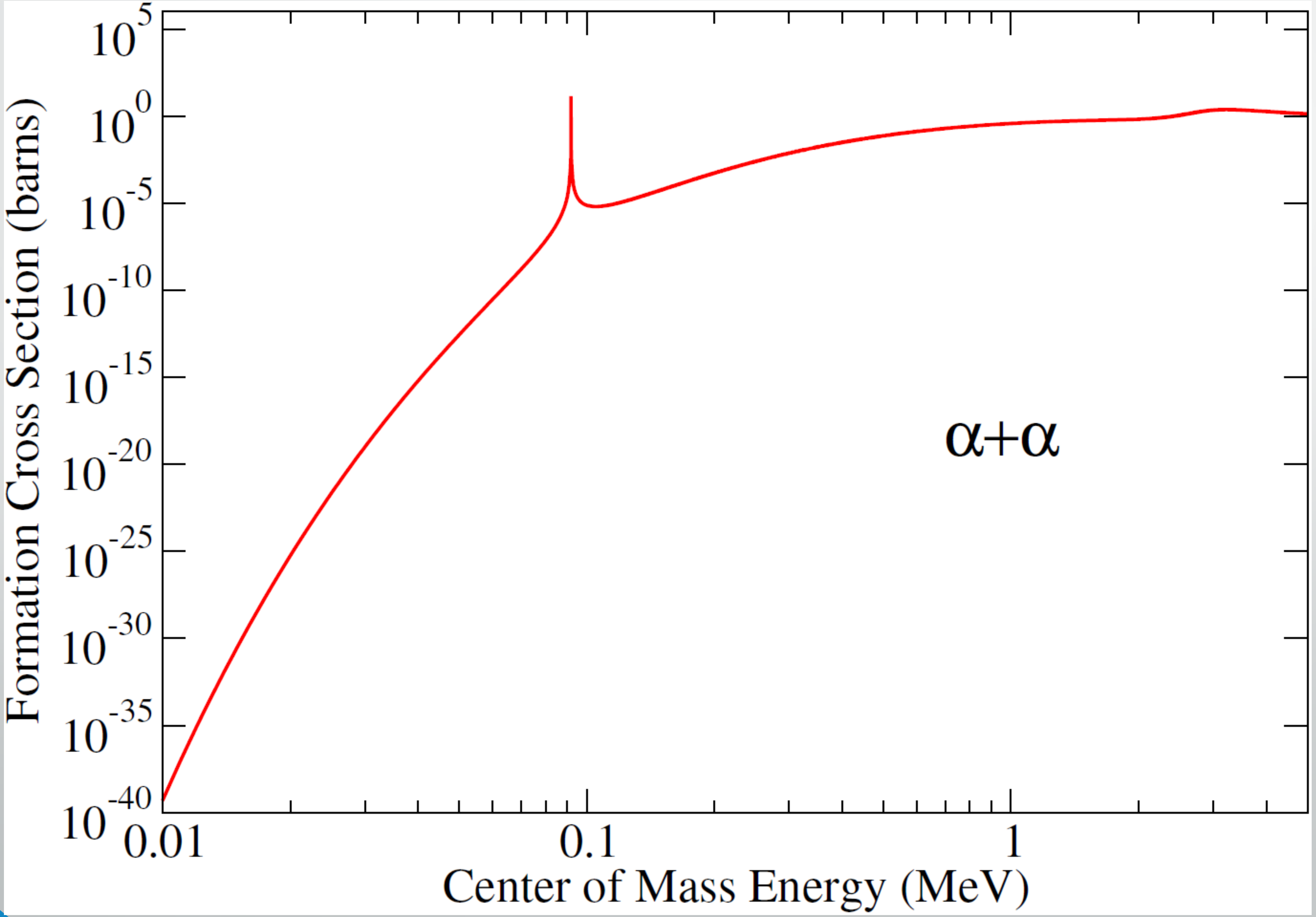


FIGURE 2 | Representation of the different roles of `emcee`, `BRICK`, and `AZURE2` in the Bayesian analysis presented below. The asterisk in the `emcee` rectangle indicates the starting point of the process.

BAND
Bayesian Analysis of Nuclear Dynamics

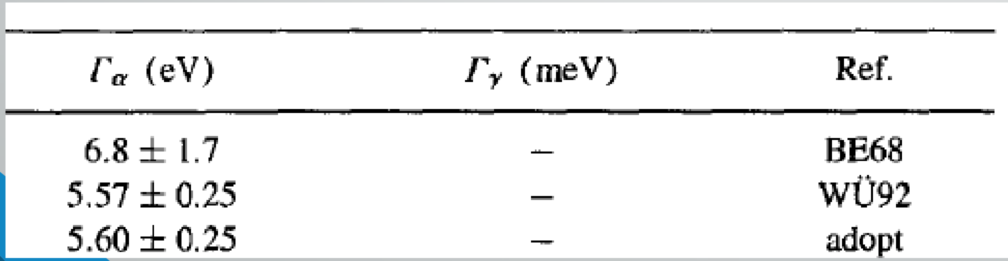
Uncertainties on the fit parameters, but more importantly the cross section and **reaction rates** are easily accessible.

α+α formation cross section

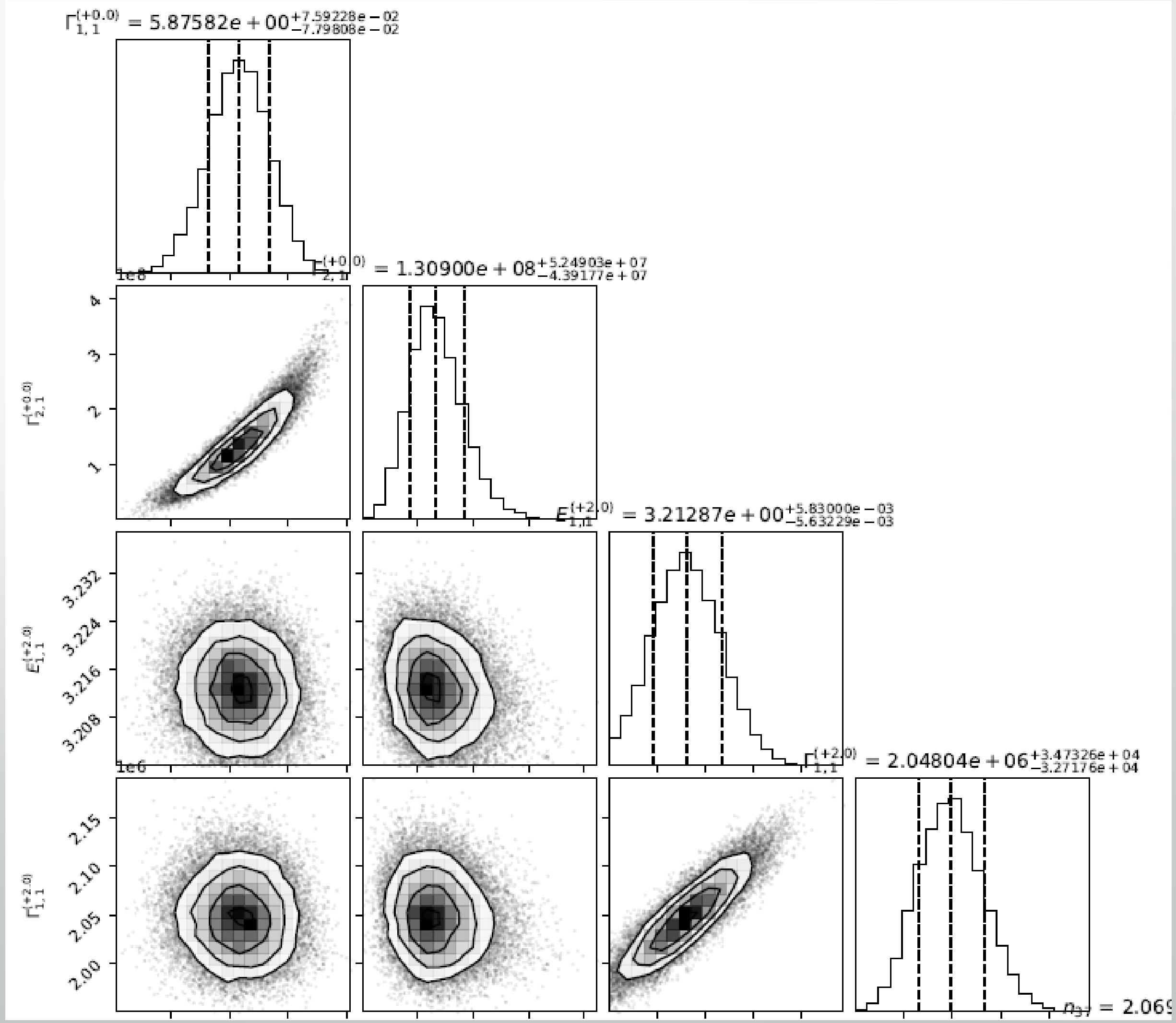


<αα>
BRICK uncertainty analysis

- MCMC sampler
  - $\Gamma_{\text{c.m.}}$ = 5.87 eV
  - Uncertainty
    - Stats --- 0.077 eV
- Other uncertainty contributions
    - Model (channel radius) --- 0.179 eV
    - Level energy --- 0.045 eV
- **$\Gamma_{\text{c.m.}}$ = 5.87(20) eV**

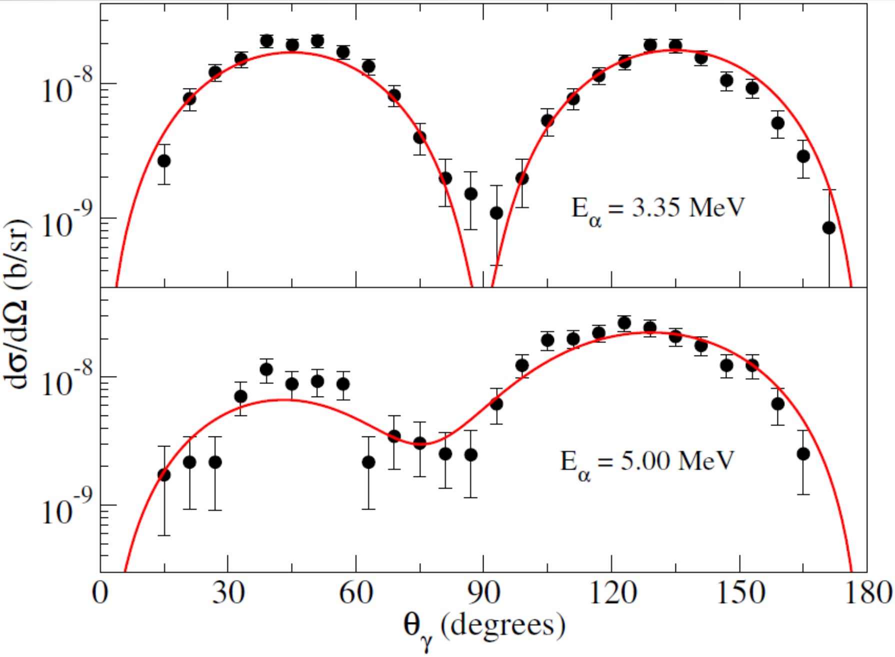


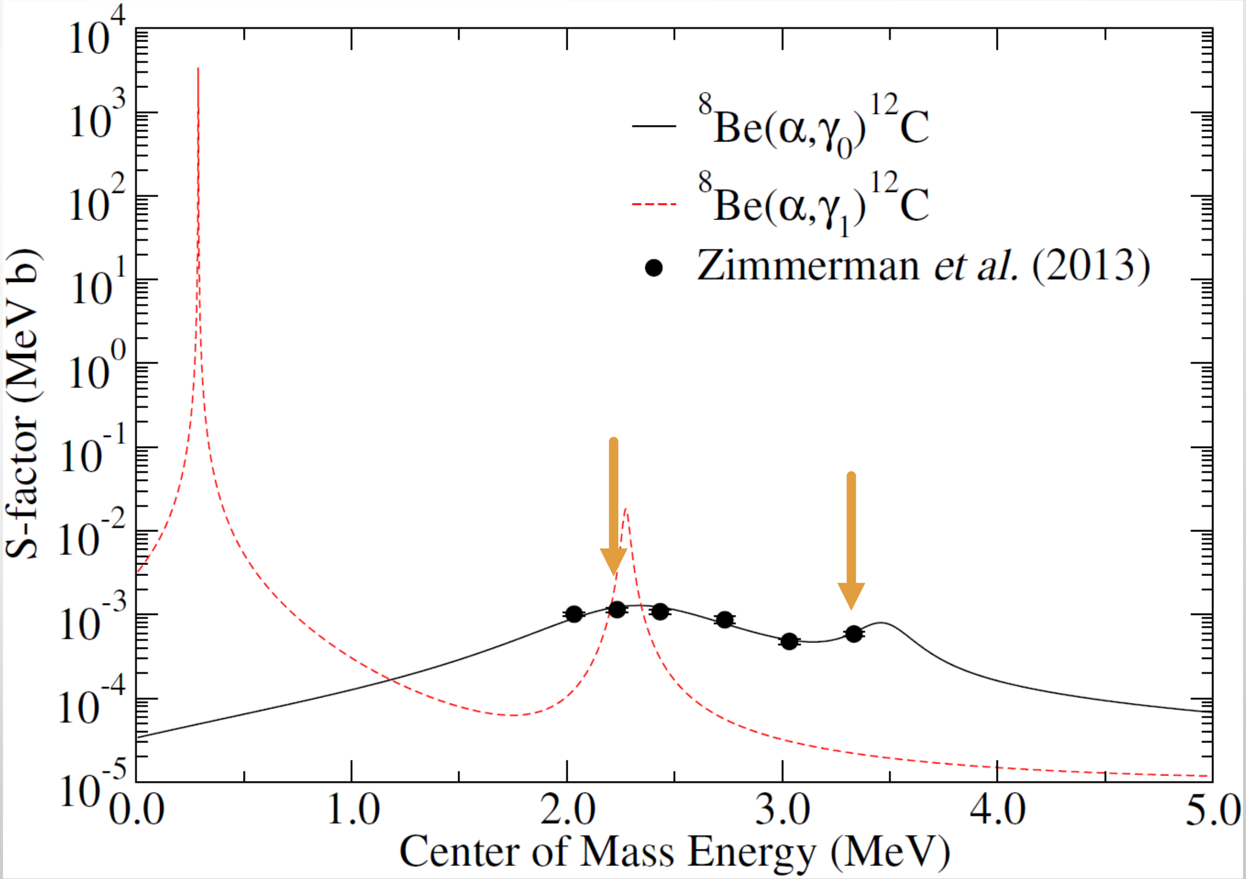
Γ_α (eV)	Γ_γ (meV)	Ref.
6.8 ± 1.7	–	BE68
5.57 ± 0.25	–	WÜ92
5.60 ± 0.25	–	adopt



^{8}Be(α,γ)^{12}C

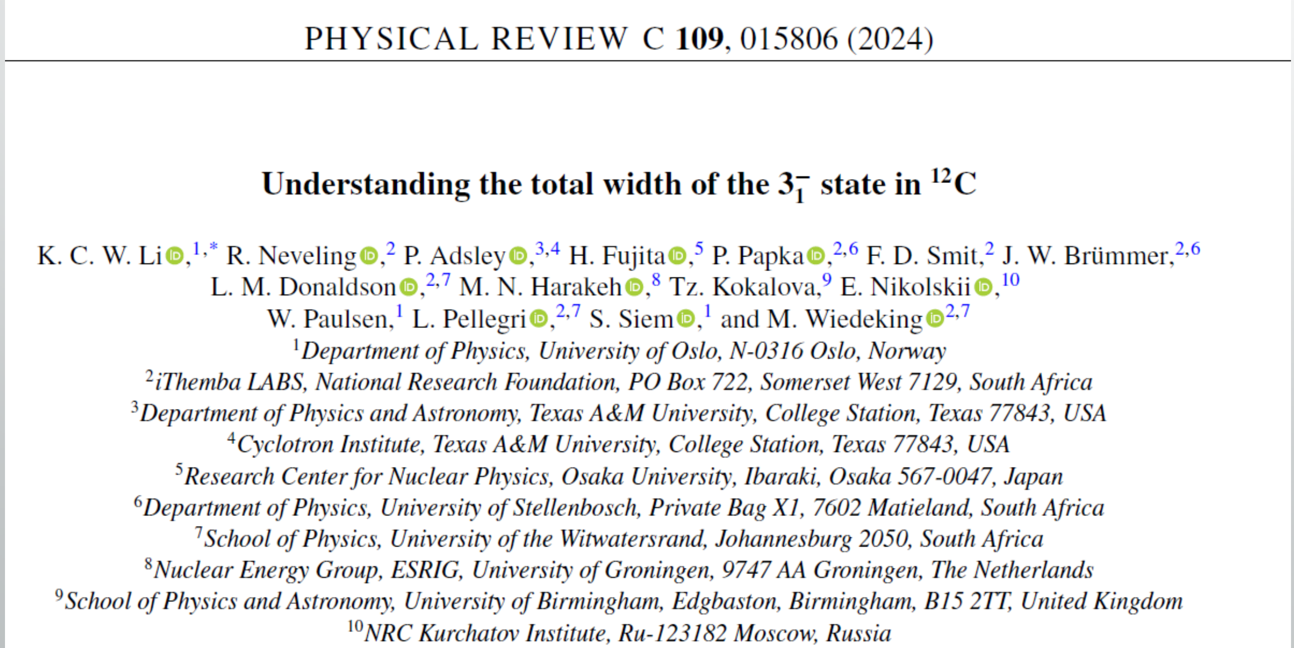
- Not a lot of higher energy data, but there is more than there used to be
- ^{12}C(γ,α_o)^{8}Be from HIγS at TUNL





<α^{8}Be>

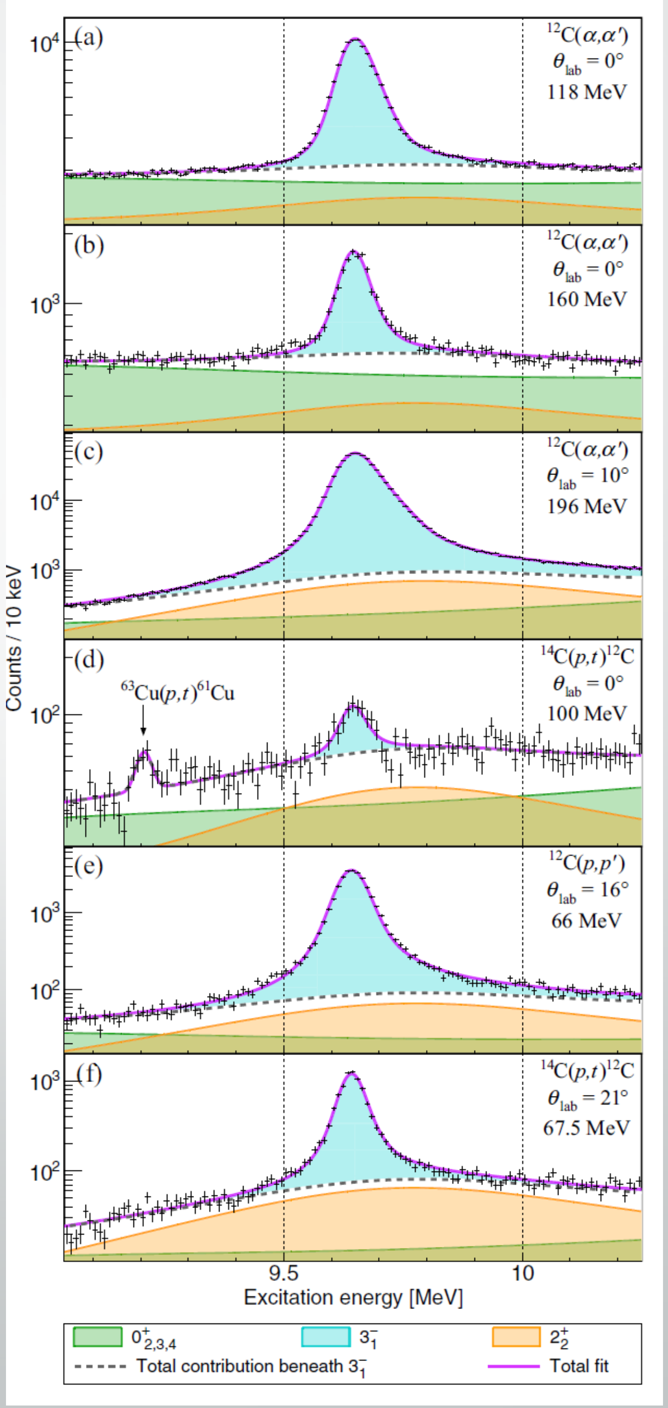
- See also recent analysis of ^{12}C(α,α′), ^{14}C(p,t)^{12}C and ^{12}C(p,p′) data
- R-matrix work by Kevin Li at University of Oslo on inelastic and transfer data also shows promise



PHYSICAL REVIEW C **109**, 015806 (2024)

Understanding the total width of the 3_1^- state in ^{12}C

K. C. W. Li,[1,*] R. Neveling,[2] P. Adsley,[3,4] H. Fujita,[5] P. Papka,[2,6] F. D. Smit,[2] J. W. Brümmer,[2,6]
L. M. Donaldson,[2,7] M. N. Harakeh,[8] Tz. Kokalova,[9] E. Nikolskii,[10]
W. Paulsen,[1] L. Pellegri,[2,7] S. Siem,[1] and M. Wiedeking[2,7]
[1] *Department of Physics, University of Oslo, N-0316 Oslo, Norway*
[2] *iThemba LABS, National Research Foundation, PO Box 722, Somerset West 7129, South Africa*
[3] *Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA*
[4] *Cyclotron Institute, Texas A&M University, College Station, Texas 77843, USA*
[5] *Research Center for Nuclear Physics, Osaka University, Ibaraki, Osaka 567-0047, Japan*
[6] *Department of Physics, University of Stellenbosch, Private Bag X1, 7602 Matieland, South Africa*
[7] *School of Physics, University of the Witwatersrand, Johannesburg 2050, South Africa*
[8] *Nuclear Energy Group, ESRIG, University of Groningen, 9747 AA Groningen, The Netherlands*
[9] *School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom*
[10] *NRC Kurchatov Institute, Ru-123182 Moscow, Russia*



External capture calculations

Langanke *et al*. (1986)

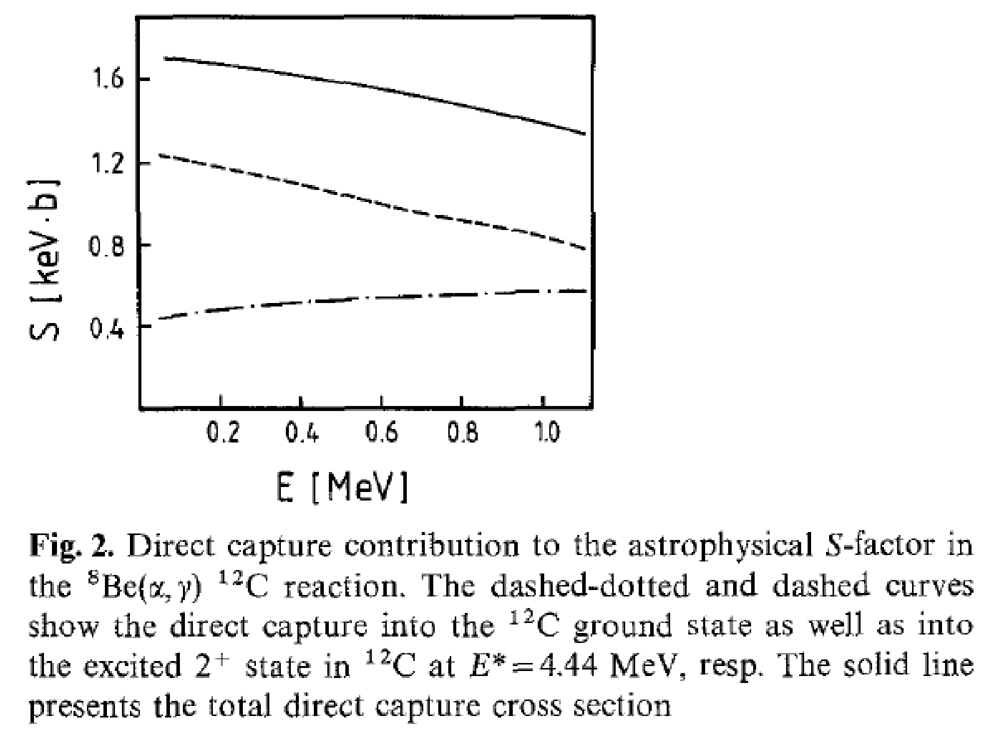
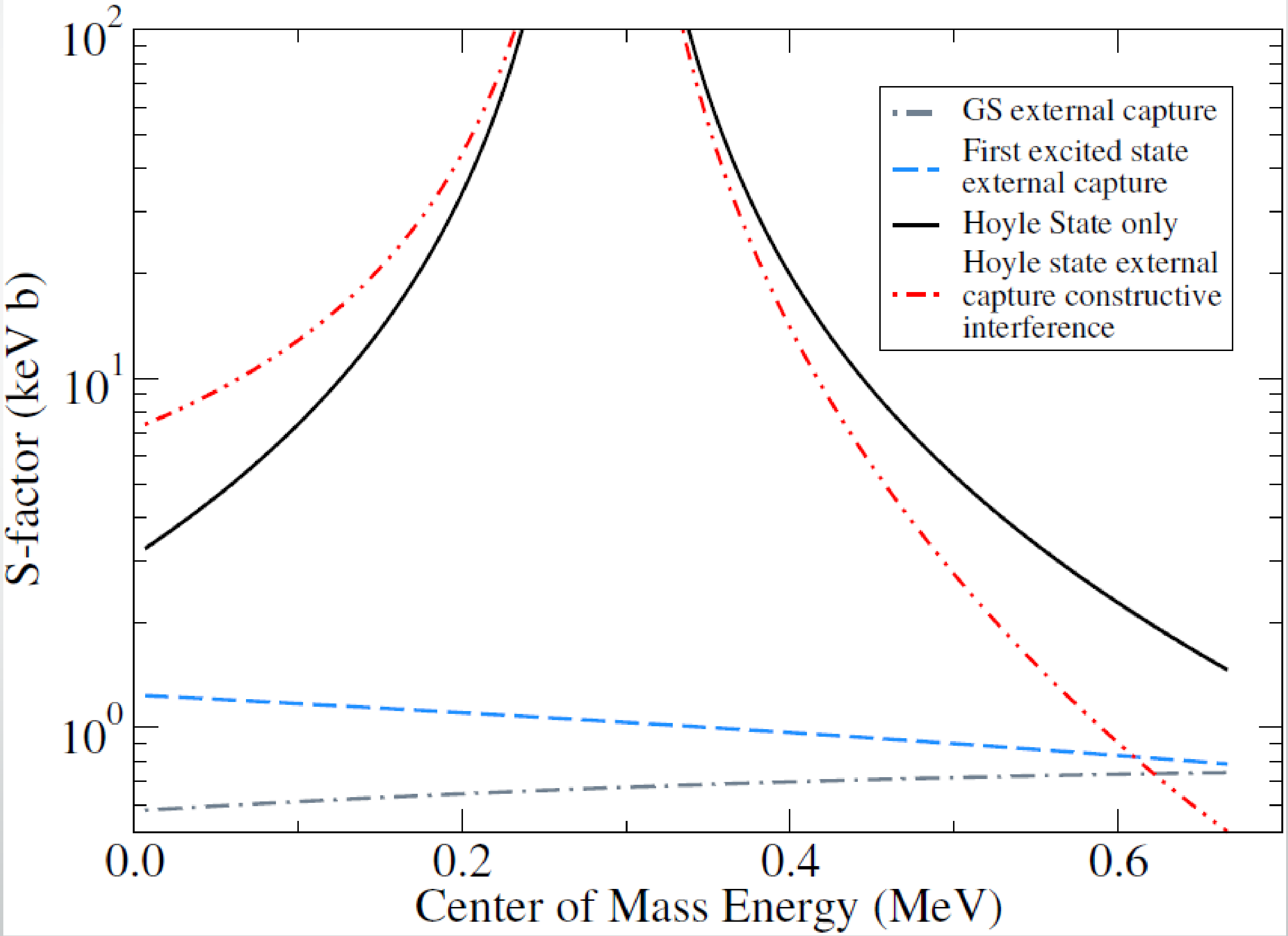
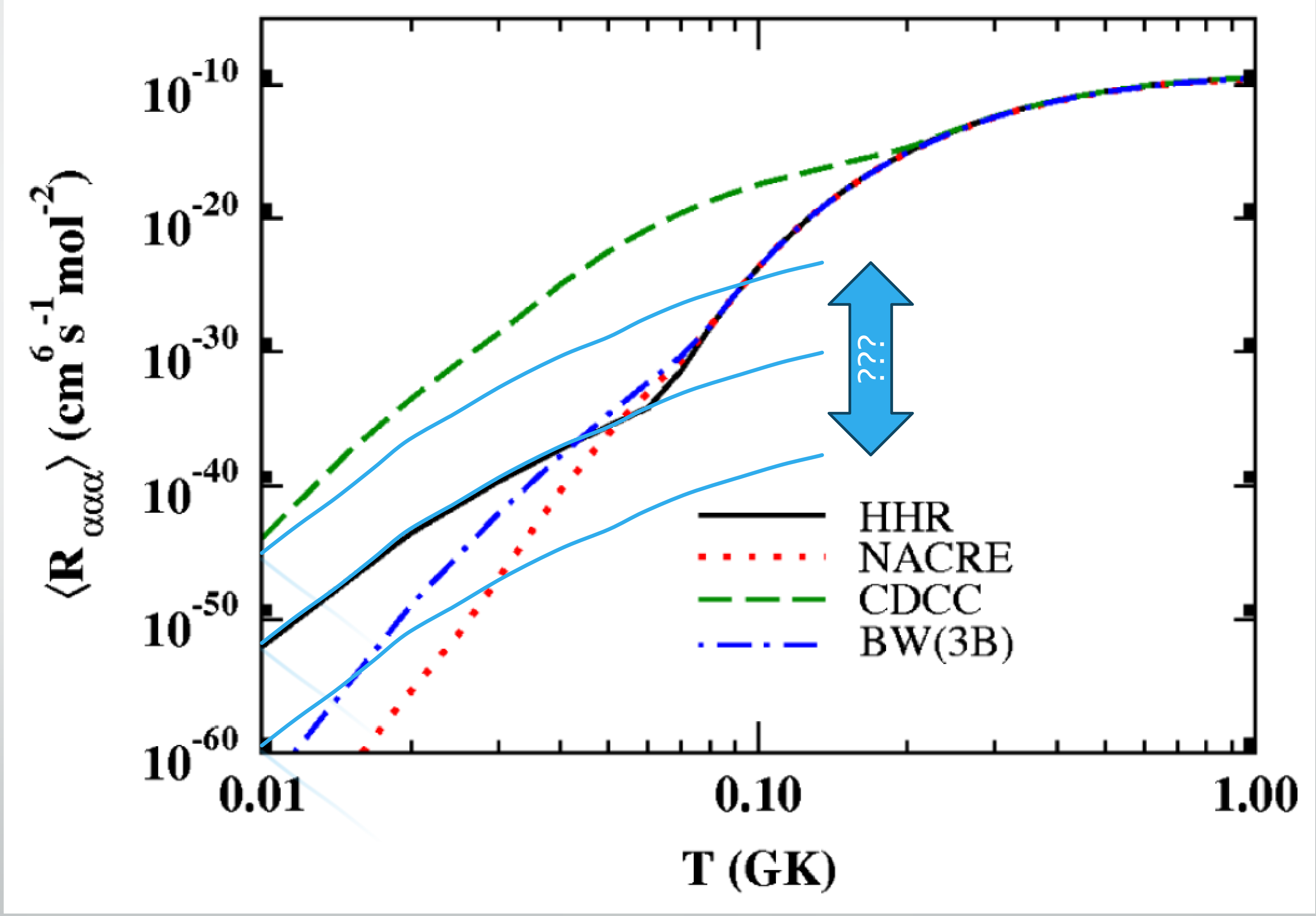


Fig. 2. Direct capture contribution to the astrophysical *S*-factor in the ^{8}Be(α,γ) ^{12}C reaction. The dashed-dotted and dashed curves show the direct capture into the ^{12}C ground state as well as into the excited 2^+ state in ^{12}C at $E^*=4.44$ MeV, resp. The solid line presents the total direct capture cross section



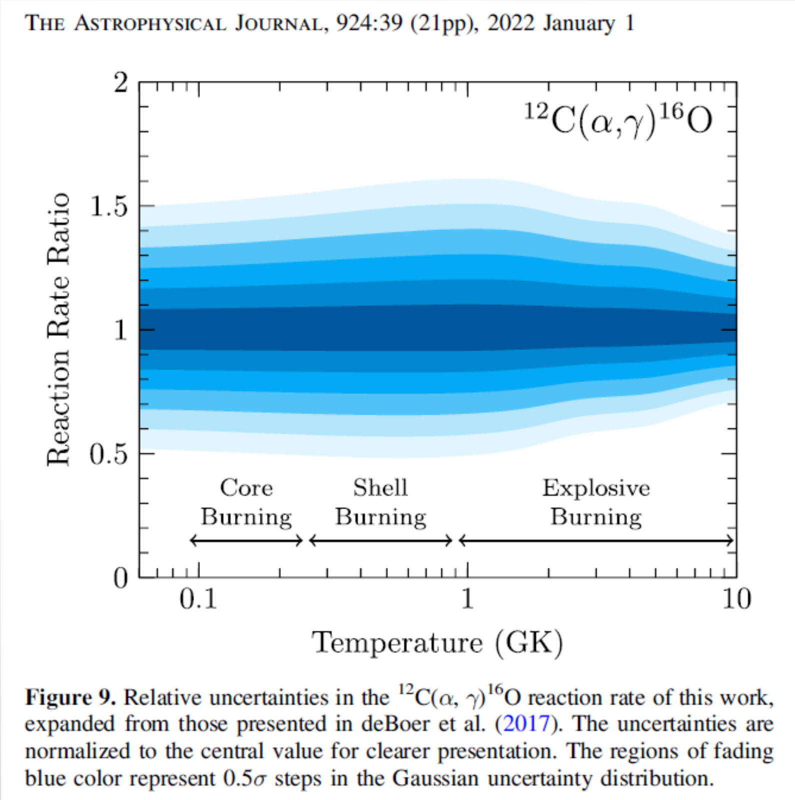
The simplest strategy

- Parameterize the temperature dependance of the 3 body rate calculation
- Estimate some uncertainty range
- What's the underlying probability distribution?
  - Hard to quantify ☹



Summary

- Still a ways to go
- R-matrix fit of $\alpha\alpha$ ground state ghost data to determine the $\Gamma_{\text{c.m.}}$ for the ^{8}Be ground state is about done
  - $\Gamma_{\text{c.m.}}$ was obtained that is consistent with that of the direct low energy analyses
- R-matrix fit for $\alpha+{}^{8}$Be has started but only for the recent HIγS data so far
- Just starting to look at how to handle the **3 body part**
  - I would like to see 3 body calculations (which include everything) decomposed into 2 body and 3 body parts
  - Daniel Phillips (OU), Carl Brune (OU) and Filomena Nunes (FRIB@MSU), Michael Wiescher (ND) and Frank Timmes (ASU) for very useful discussions!



The Astrophysical Journal, 924:39 (21pp), 2022 January 1

Figure 9. Relative uncertainties in the ^{12}C(α, γ)^{16}O reaction rate of this work, expanded from those presented in deBoer et al. (2017). The uncertainties are normalized to the central value for clearer presentation. The regions of fading blue color represent 0.5σ steps in the Gaussian uncertainty distribution.

This, but for 3α

In the works