Applications of R-matrix Methods to Light Nuclei

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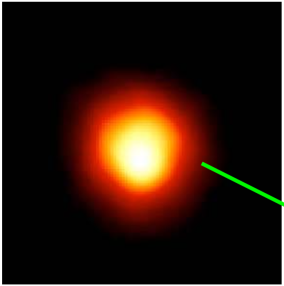
What is R-matrix ?

- A scheme for describing nuclear reactions using a basis defined inside a channel radius.
- It is well suited for phenomenology (data evaluation).
- As much quantum mechanics as possible is put in:.
  - Angular momentum and parity conservation.
  - Long-range Coulomb interaction.
  - Probability conservation (unitarity).
  - Time-reversal invariance.

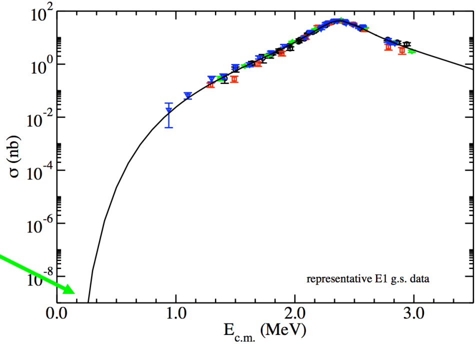
The Challenge

Red Giant



$T=(1\text{-}3)\text{x}10^8$ K

The Lab



- Extrapolation of $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$ to low energies is required. More challenging than the typical data evaluation problem.

Some Important Literature for Nuclear Reaction Phenomenology with R-Matrix

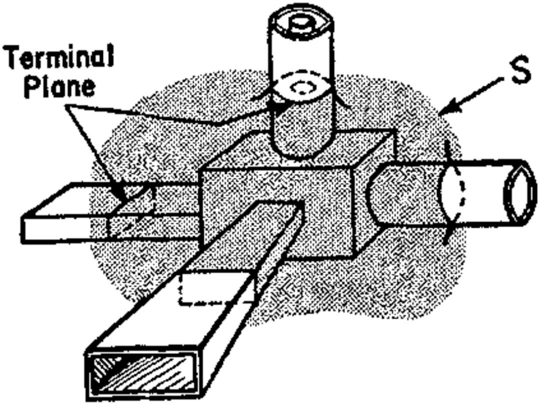
Original Literature

- G. Breit and E. Wigner, *Capture of Slow Neutrons*, Phys. Rev. **49**, 519-531 (1936).
- P.L. Kapur and R. Peierls, *The dispersion formula for nuclear reactions*, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, **166**, Issue 925, pp. 277-295, (1938).
- A.J.F. Siegert, *On the Derivation of the Dispersion Formula for Nuclear Reactions*, Phys. Rev. **56**, 750-752 (1939).
- E.P. Wigner and L. Eisenbud, *Higher Angular Momenta and Long Range Interaction in Resonance Reactions*, Phys. Rev. **72**, 29-41 (1947).
- C. Bloch, *Une formulation unifiée de la théorie des réactions nucléaires*, Nucl. Phys. **4**, 503-528 (1957).
- A.M. Lane and D. Robson, *Comprehensive Formalism for Nuclear Reaction Problems. I. Derivation of Existing Reaction Theories*, Phys. Rev. **151**, 774-787 (1966).
- F.C. Barker, *The boundary condition parameter in R-matrix theory*, Australian Journal of Physics **25**, 341-348 (1972).
- G.M. Hale, R.E. Brown, and N. Jarmie, *Pole structure of the* $J^\pi = 3/2^+$ *resonance in* ^{5}He, Phys. Rev. Lett. **59**, 763-766 (1987).
- C.R. Brune, *Alternative parametrization of R-matrix theory*, Phys. Rev. C **66**, 044611 (2002).

Review Articles

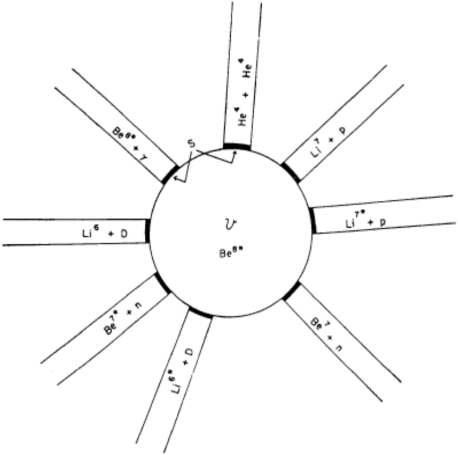
- A.M. Lane and R.G. Thomas, *R-Matrix Theory of Nuclear Reactions*, Reviews of Modern Physics **30**, 257-353 (1958).
- P. Descouvemont and D. Baye, *The R-matrix theory*, Reports on Progress in Physics **73**, 036301 (2010).
- R.J. deBoer, CRB *et al.*, The ^{12}C$(\alpha,\gamma)^{16}$O reaction and its implications for stellar helium burning, Reviews of Modern Physics, **89**, 035007 (2017).

An Intuitive Picture for Nuclear Reactions



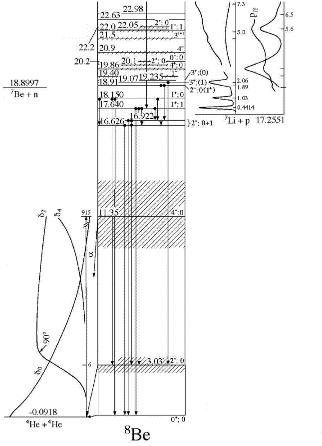
"A transmission line (waveguide) junction"
E.P. Wigner, *Nuclear Reactions and Level Widths*,
American Journal of Physics **17**, 99-109 (1949).

Making the Picture more Nuclear



"Resonance Reactions"
E. W. Vogt, in Nuclear Reactions, Vol. 1,
edited by P. M. Endt and M. Demeur
(North-Holland, Amsterdam, 1959).

Example of Channels: ^{8}Be



http://www.tunl.duke.edu/nucldata/

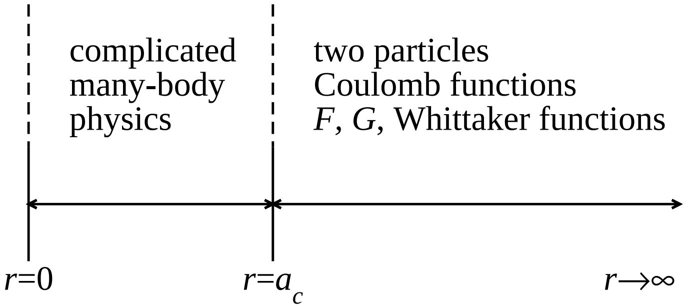
spins and parities:

"particle"	J	π
p	1/2	+
^{4}He	0	+
^{7}Li	3/2	-
^{7}Li*(0.48)	1/2	-

channels

α	s	ℓ	J	π
^{4}He + ^{4}He	0	0	0	+
^{4}He + ^{4}He	0	2	2	+
$p + {}^7$Li	1	0	1	-
$p + {}^7$Li	2	0	2	-
$p + {}^7$Li	1	1	0,1,2	+
$p + {}^7$Li	2	1	1,2,3	+
$p + {}^7$Li*(0.48)	0	0	0	-
$p + {}^7$Li*(0.48)	1	0	1	-
$p + {}^7$Li*(0.48)	0	1	1	+
$p + {}^7$Li*(0.48)	1	1	0,1,2	+

Basic Idea of the R-Matrix Approach



- Inside the channel radii, a basis of states is used, with each state corresponding, more or less, to an energy level.
- The basis must be truncated, depending upon the available data.

The R Matrix

- Working inside the channel radius allows a discrete basis $|\lambda\rangle$ to be utilized.
- Bound and scattering states enter on equal footing. R-matrix theory is an ideal tool for threshold physics.
- In the Wigner-Lane-Thomas (WLT) implementation, the basis is taken to be eigenfunctions characterized by energies E_λ that satisfy a particular boundary condition at the channel radius (real, constant, and energy-independent radial log-derivative).
- The R-matrix is then defined to be

$$R_{c'c} = \sum_\lambda \frac{\gamma_{\lambda c'}\gamma_{\lambda c}}{E_\lambda - E}.$$

- The reduced widths $\gamma_{\lambda c}$ are the projections of the eigenfunctions on to the two-body channel c at the channel radius.

The R Matrix, continued

- Note that $\boldsymbol{R}$ depends on E, the excitation energy in the compound nucleus.
- The scattering matrix $\boldsymbol{S}$ may now be calculated from the $\boldsymbol{R}$ matrix and Coulomb functions evaluated at the channel radii. I will skip the formulas.
- One may think about this as

$$R \text{ Matrix} \rightarrow S \text{ Matrix} \rightarrow \text{Scattering Amplitudes} \rightarrow \text{Observables}$$

- It is remarkable that we don't need the full basis functions – just their energies E_λ and amplitudes at the channel radii $\gamma_{\lambda c}$.

Phenomenological R Matrix

- Adjust E_λ and $\gamma_{\lambda c}$ to describe data!
- These parameters are (mostly) related to to the level energies partial widths of those levels.
- Interestingly, observable quantities, i.e., the S matrix, only depend upon a few properties of discrete eigenfunctions: the energy eigenvalues and the amplitudes at the channel radii.
- The numbers of levels and channels must be truncated.
- Fortunately, the truncations in levels and channels do no destroy the unitarity and time-reversal invariance properties of the S matrix. This is a key reason why the phenomenological R-matrix approach is so useful.

Power of the S Matrix

- The phenomenological R-matrix automatically yields an S-matrix with the necessary unitary and symmetric properties.
- This property links data in different reaction channels to the same R-matrix parameters.
- Furthermore, the Breit-Wigner formula or its R-matrix generalization links the widths of resonances to their height or strength – thus reducing the uncertainty in the absolute cross section.
- This is how you beat the spline fit!

R-matrix versus alternatives

- Effective Range Theory and the modified K-matrix are alternatives.
- Effective Range Theory is not a natural tool for resonances.
- One advantage of R-matrix is that it is related to a basis:
  – parameters can be connected to wave functions
  – truncation is easier to evaluate
  – isospin and mirror symmetry can be implemented
  – perturbation theory can be applied:
    γ decays, β decays, transfer reactions,...

When and Why to use Phenomenological R-matrix

- Ab initio or other theoretical approaches may
  - lack the desired precision
  - not be possible
- Parametrization of data for applications: astrophysics, etc…
- Extrapolation / interpolation of data into regions without data
- When dealing with resonances
  - particularly when dealing with more than one
  - particularly when resolved with widths are non-negligible
    - $\rightarrow A < 25$
    - $\rightarrow$ neutron-induced reactions at low energies
  - The Hauser-Feshbach formula may be derived from R-matrix
- Low energies (few channels)
- When incorporating information from multiple sources:
  - cross section data
  - spectroscopic information (excitation energy, spin,…)
  - transfer reactions (ANCs, spectroscopic factors)
  - theoretical calculations

Choosing the Channel Radius

- Formally, the channel radii should be chosen large enough so that nuclear interactions have become negligible.
- However, in a phenomenological analysis, using channel radii which are "too large" cause problems: the states corresponding to a particle in spherical box start coming into play.
- In practice, one typically wants to use a radius just a little bit larger than the "surface" of the nucleus.
- $a_c = 1.4(A_1^{1/3} + A_2^{1/3})$ fm is a reasonable starting point.
- The sensitivity of any conclusions to the adopted radii should be investigated. A large sensitivity indicates that the number of levels has been overly truncated and that an additional (background) level should be included.
- Because there may be some nuclear interactions beyond the radii used in practice, the $\gamma_{\lambda c}$ should be considered to be renormalized quantities, that do not necessarily correspond exactly to the true wavefunction at the channel radii.

R-Matrix Boundary Conditions

The boundary conditions define the basis:

- $\rho \frac{u'}{u} |_{r=a} = B$ real, energy-independent $\rightarrow$ real E_λ, γ_λ
  Wigner, Lane, Thomas,… The basis vectors are orthogonal inside the channel radius.
- $\rho \frac{u'}{u} |_{r=a} = S(E)\,|_{r=a}$ real, energy-dependent $\rightarrow$ real E_λ, γ_λ
  Helps with interpretation of parameters, equivalent to above. The basis vectors are not orthogonal inside the channel radius.
- $\rho \frac{u'}{u} |_{r=a} = [S(E) + iP(E)]_{r=a}$ complex, energy-dependent $\rightarrow$ complex E_λ, γ_λ. Kapur and Peierls (1938), Siegert (1939): Gamow / Siegert states. Simple relationship to S matrix, but does not seem to be a practical basis for fitting data.

In all of the above, E_λ and γ_λ also define poles and residues of a matrix (R, R_S, or S).

Alternative parametrization

- The energies and reduced widths in the traditional WLT approach are related to the actual energy levels and partial widths in a very complicated way.
- One can redefine the parameters E_λ and $\gamma_{\lambda c}$ so that they correspond to $B_c(E_R) = S_c(E_R)$ for all levels.
  See CRB, Phy. C **66**, 044611 (2002)
  `https://doi.org/10.1103/PhysRevC.66.044611` .
- This approach is known as the alternative or Brune basis.
- This is what is done by default in the AZURE2 code.

Features of the alternative basis

- It is mathematically equivalent to the Lane-and-Thomas formalism.
- Level shifts are eliminated, so that exact excitation energies can be easily implemented.
- Interpretation of fit parameters in terms of excitation energies, partial widths, and/or ANCs is straightforward.
- Parameter correlations are reduced. This feature is important for fitting and/or random-walk parameter searching.
- This parametrization was recently re-derived in a paper by Park, Phys. Rev. C **104**, 064612 (2021). There is nothing new in this paper.

R-Matrix Computer Codes

- For simple problems, you might consider programming it up yourself.
- There are many codes in use, including `SAMMY` and `EDA`. I can also recommend the `AZURE2` code: https://azure.nd.edu
- AZURE: An R-matrix code for nuclear astrophysics, R. E. Azuma, E. Uberseder, E. C. Simpson, C. R. Brune, H. Costantini, R. J. de Boer, J. Görres, M. Heil, P. J. LeBlanc, C. Ugalde, and M. Wiescher, Phys. Rev. C 81, 045805, 17 pages (2010). https://doi.org/10.1103/PhysRevC.81.045805
- Uses the *alternative basis*, see Carl Brune, Phys. Rev. C **66**, 044611, (2002). https://doi.org/10.1103/PhysRevC.66.044611
- Specifically designed for nuclear astrophysics applications.
- Includes the external contribution to radiative capture in the Barker-Kajino formalism.

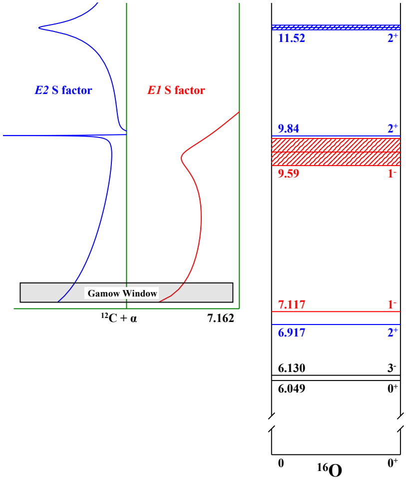
$^{12}C(\alpha,\gamma)^{16}O$: Important Energy Levels

Physics: Subthreshold resonances and interference

Note: Subthreshold resonances along with their interference is required to obtain $S(300)$.

S factor: $\sigma = \frac{S}{E}\exp(-2\pi\eta)$

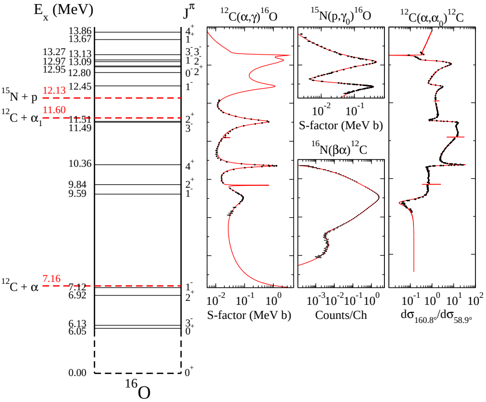
$$\eta = \sqrt{\frac{\mu}{2E}} Z_1 Z_2 \frac{e^2}{\hbar^2}$$



A partial level diagram

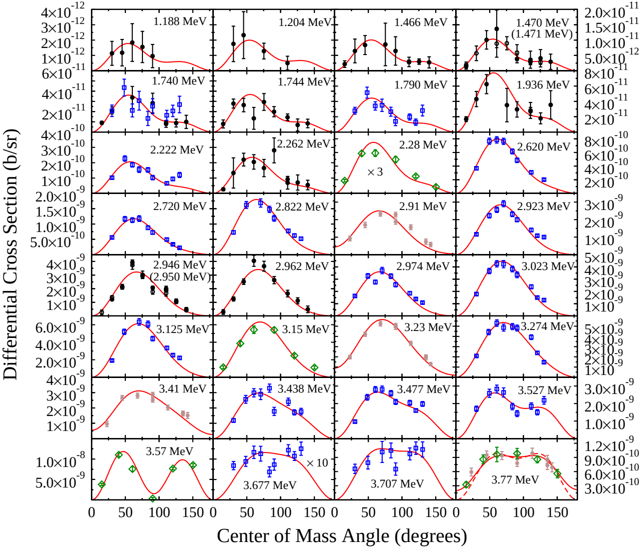
Global R-Matrix Analysis

Reviews of Modern Physics **89**, 035007 (2017)



- James deBoer (leader), R.E. Azuma, A. Best, C.R. Brune C.E. Fields, J. Görres, S. Jones, M. Pignatari, D. Sayre, K. Smith, F.X. Timmes, E. Uberseder, and M. Wiescher. https://doi.org/10.1103/RevModPhys.89.035007
- $> 15,000$ data points fitted.
- Bound state information (E_x, Γ_γ, ANCs) also included.

Fits to Ground-State $^{12}C(\alpha,\gamma)$ Angular Distributions



Dyer and Barnes (1974, green diamonds), Redder *et al.* (1987, brown stars), Assunção *et al.* (2006, black circles), Fey (2004, blue squares).

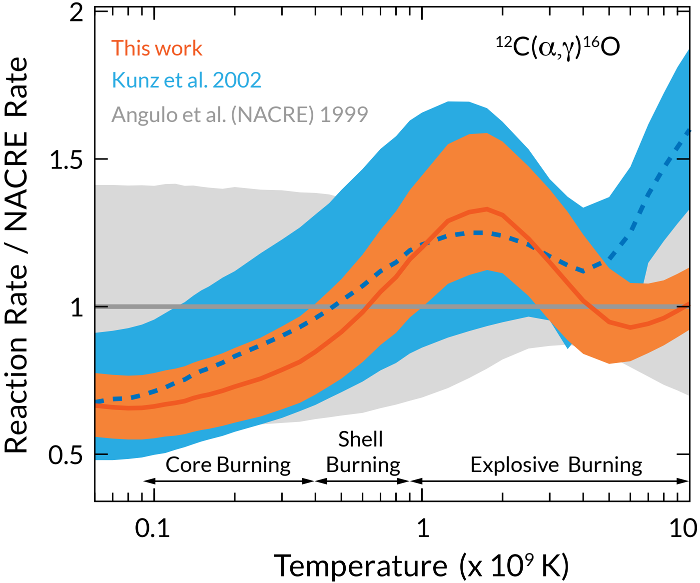
Summary of Results at $E = 300$ keV

- $E1$ ground-state S factor: 86 keV-b
- $E2$ ground-state S factor: 45 keV-b
- Cascade S factor: 7 keV-b

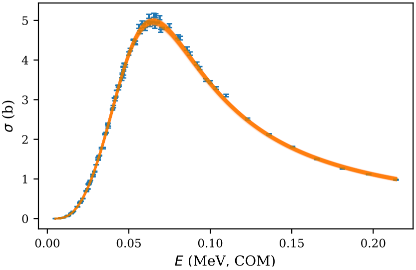
- Total S factor: 140 keV-b
- Estimated Uncertainty:

± 14	data (Monte Carlo)
$+18/-11$	model

Reaction Rate

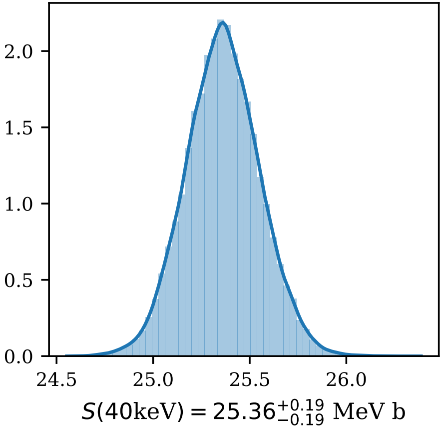


The ^{3}H$(d,n)^4$He Reaction at Low Energies



- Important for Big-Bang Nucleosynthesis and fusion applications.
- Data considered: Conner *et al.* (1952), Arnold *et al.* (1953), Kobzev *et al.* (1966), Jarmie *et al.* (1984), Brown *et al.* (1987).
- Bayesian analysis by Daniel Odell, Carl Brune, and Daniel Phillips, Phys. Rev. C **105**, 014625 (2022). https://doi.org/10.1103/PhysRevC.105.014625

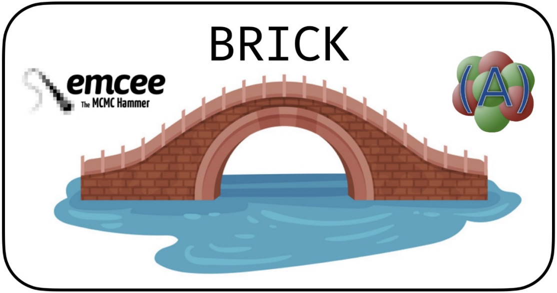
The ^{3}H$(d,n)^4$He, continued



- With Bayesian Monte Carlo sampling, it is straightforward to study the posterior probability distribution of any calculated quantity.

Bayesian R-matrix Inference Code Kit (BRICK)

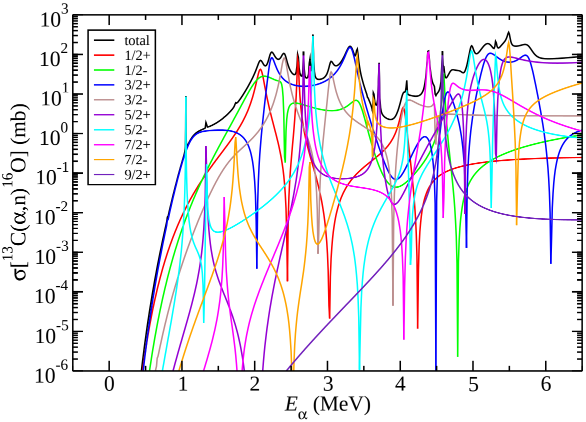
- BRICK is a python software package (https://github.com/odell/brick) that interfaces R-matrix and calculations Monte Carlo sampling.
- R-matrix: AZURE2, http://azure.nd.edu
- Sampling: emcee, https://github.com/dfm/emcee



Bayesian versus χ^2 fitting

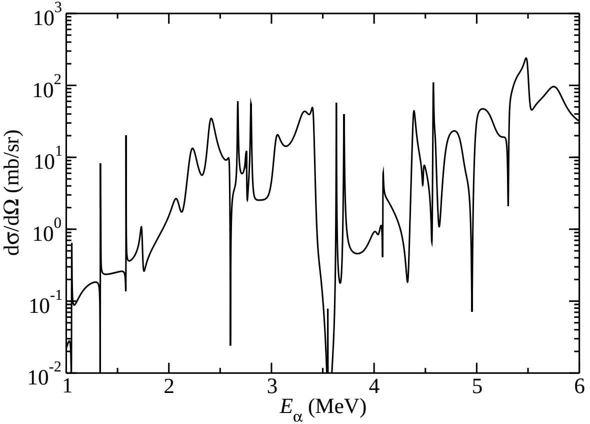
- Bayesian:
  - fine-grained modeling of errors
  - simple error estimation for any calculated quantity
  - computationally demanding
- χ^2 minimization:
  - essentially limited to uncorrelated Gaussian errors
  - emphasis on goodness of fit

The $^{13}C(\alpha, n)^{16}O$ Reaction



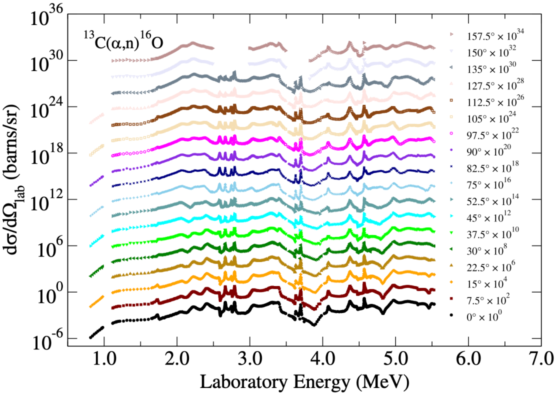
- Important s-process neutron source and, via the time-reverse reaction, a neutron sink water-moderated power reactors.
- Partial wave decomposition of the $^{13}C(\alpha, n)$ cross section, as implemented in the 2018 ENDF/B-VIII evaluation by Hale and Paris (LANL) using their `EDA` code.

The $^{13}\mathrm{C}(\alpha, n)^{16}\mathrm{O}$ Reaction, continued



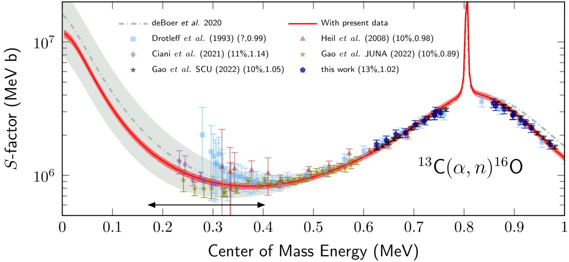
- The curve shows the 2018 ENDF/B-VIII prediction for the 0° differential cross section, by Hale and Paris (LANL) using their `EDA` code.

The $^{13}C(\alpha,n)^{16}O$ Reaction, continued



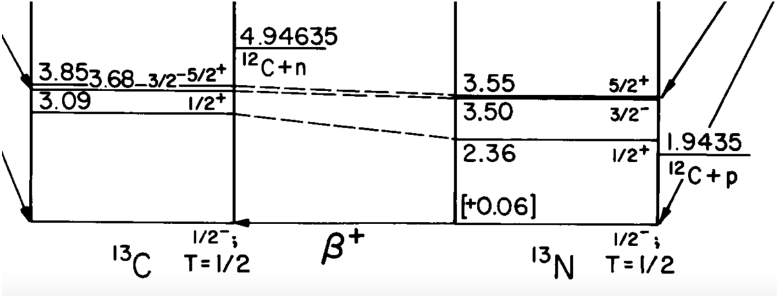
- There has been a lot of recent work on this reaction, over a wide range of energies.
- One nice new measurement has been conducted at Notre Dame using deuterated scintillators: R.J. deBoer *et al.*, Phys. Rev. Lett. **132**, 062702, (2024). https://doi.org/10.1103/PhysRevLett.132.062702

The $^{13}\mathrm{C}(\alpha, n)^{16}\mathrm{O}$ Reaction, continued



- The measurements help to determine the "background" levels at higher energies, making the low-energy extrapolation more accurate.
- $\approx \times 2$ reduction in uncertainty for $T = 0.2$ GK.

Isospin and Mirror Symmetry: $A = 13$ Isobar Diagram



http://www.tunl.duke.edu/nucldata/

Can we understand why levels are bound in ^{13}C but unbound in ^{13}N?

Thomas-Ehrman Shift

- Use the R-matrix idea: the wavefunctions are about the same inside the channel radius.
- This suggest the logarithmic derivatives should be the same.
- What does this say about the separation energy?
- The separation energies (energies relative to threshold) must be different!
- See J.B. Ehrman, Phys. Rev **81**, 412 (1951) and R.G. Thomas, Phys. Rev **88**, 1109 (1952).
- The reduced width of the level is also important. The effect is largest when the reduced width in threshold channel is large and $\ell = 0$.
- A full understanding of such energy differences is quite complicated, and still an interesting research topic.

PROC. PHYS. SOC., 1964, VOL. 84

A model for nuclear threshold levels

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MS. received 30*th June* 1964

Abstract. The observation of some levels in light nuclei closer to thresholds than one might expect from average level densities suggests the investigation of models which might produce such an effect. One model based on the *R*-matrix theory of nuclear reactions is shown to predict that near thresholds of channels with small barriers there should be an increased density of levels with large reduced widths. The experimental evidence for such an effect is meagre.

What is the idea here?

- Energy levels have a boundary condition requirement outside the nuclear surface: exponential decay (bound states) or some version of an outgoing wave (unbound states).

- Near a threshold, this condition is strongly non-linear in energy and leads an "attraction" of levels to the threshold. The effect may also be termed "excitation energy compression."

- The effect is strongest for low orbital angular momentum and when the wavefunction has a large component in the two-body channel which has a nearby threshold.

- There are many examples of great practical significance:
  fusion [$^{3}\mathrm{H}(d,n)^{4}\mathrm{He}$, $^{3}\mathrm{He}(d,p)^{4}\mathrm{He}$],
  neutron detection [$^{3}\mathrm{He}(n,p)^{3}\mathrm{H}$, $^{6}\mathrm{Li}(n,t)^{4}\mathrm{He}$, $^{10}\mathrm{B}(n,\alpha)^{7}\mathrm{Li}$],
  and astrophysics [$^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$,...].

Multiple levels with the same J^π

- The outgoing wave boundary condition satisfied by the bound or resonant states breaks isospin.
- The constant boundary condition of Wigner, Lane, Thomas,... (WLT) basis does not.
- $\rightarrow$ apply isospin in the WLT basis. This includes an energy shift and changes in charges.

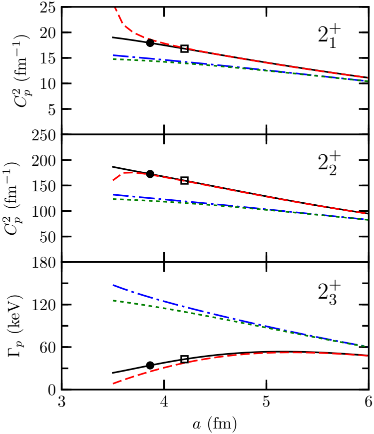
Multiple levels with the same J^π, continued

- These basis changes involve linear (and sometimes non-linear) algebra.
- The relative signs of the reduced-width amplitudes are required. These may be taken from a shell-model calculation or treated as an uncertainty.
- This leads to a mixing of the physical states across the multiplet.
- This also provides the multi-level generalization of the Thomas-Ehrman shift.

2^+ states of ^{18}O and ^{18}Ne

- The proton ANC of the 2_2^+ state of ^{18}Ne is important for determining the $^{17}\mathrm{F}(p,\gamma)^{18}$Ne reaction rate in the hot CNO cycle.
- There is also a striking (apparent) isospin violation for the 2_3^+ states of ^{18}O – ^{18}Ne that is well-established experimentally.
- See CRB, Phys. Rev. C **102**, 034328 (2020), `https://doi.org/10.1103/PhysRevC.102.034328` .

predictions in ^{18}Ne from measured ^{18}O ANCs:



blue, green: naive mirror symmetry

red, black: multi-level mirror symmetry

Testing the phenomenological R-matrix

The phenomenological R-matrix requires the use of channel radii that enclose most, but not all, of the nuclear interactions. Background poles are also necessary because of truncation. How does one test these aspects of the theory?

- Ab initio calculations for light nuclear systems are now available, e.g. for $\alpha + d$ scattering and the ^{6}Li bound state. These are in some sense "perfect data."
  - What are the limiting factors on fit accuracy?
  - Can bound state properties be extracted from scattering data?

- One can include a phenomenological tail of the nuclear potential in the R-matrix analysis. What effect does this have on the quality of it, channel radius sensitivity, and other conclusions?

Open questions / future

- Extension to higher energies:
  - Merge with Hauser Feshbach
  - Allow certain parameters to be complex
- Photon channels:
  - External capture (perturbation theory)
  - Reich-Moore
  - Photon wavefunctions
- Three-body channels

Thank you for your attention.