Improving Astrophysical Nuclear Rates with New Many-Body & Fewer-Body Reaction Models

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Quick summary of nuclear reaction theory for astrophysics

Astrophysical nuclear reaction/scattering theory is many things:

1. Direct (radiative or nonradiative) reactions – nonresonant
   ($A \lesssim 12$ & near closed shells)

2. Reactions through isolated resonances – $12 \lesssim A \lesssim 30$

3. Reactions at high level density – heavier nuclei mid-shell or far from stability

Phenomenological R-matrix is the right way to approach Case 2

Probably Case 3 will always lean on broad systematics (functions of (A, Z))

I'll talk about Case 1: Precision is needed for BBN & solar ν's

Direct reaction theory: typical ingredients

Most methods involve 2 or 3 bodies with effective potentials

Potential shape usually comes from systematics in (A, Z) & depth is tailored to system modeled

"Spectroscopic factor" of the restricted 2- or 3-body space comes from shell model or normalization to data

This stuff has served nuclear physics & astrophysics well

But it won't deliver $\sim 1\%$ error (for BBN, solar ν's)

Until recently, computational limitations kept nucleon-level models from being significantly better

Quick survey of *ab initio* theory

For bound & narrow states at low A there is now well-developed *ab initio* theory

Starting point is a quantitatively accurate potential describing NN scattering

Off-shell & 3-body terms of potential must come from nuclei, but starting point is honestly nucleon-level

Several approaches exist (Green's function Monte Carlo, fermionic molecular dynamics, no-core shell model, lattice Monte Carlo, coupled cluster...)

Low-lying discrete states are well-computed at $A \lesssim 20$, favorable cases out to $A \sim 100$

Making the *ab initio* continuum tractable

Initial work on *ab initio* scattering & reactions has focused on making it resemble bound states

Either:

Discretize the continuum for diagonalization or energy minimization (GFMC, NCSM, Gamow shell model, fermionic molecular dynamics)

Or:

Project many-body Schrödinger equation into a 2-cluster Schrödinger-like equation in the desired channel (NCSMC/RGM, lattice EFT)

A lot has been done with nucleon scattering in NCSMC & RGM, but NNN terms & α scattering are still in early days

Lippmann-Schwinger & related approaches

But Lippmann-Schwinger (integral) formalism generally handles scattering/reaction boundary conditions better

$$\Psi^{(+)} = \Psi_0 + \Big(E - H + i\epsilon)^{-1} V \Psi_0$$

A lot of the *ab initio* future probably belongs to integral-equation approaches

I've started with "Lippmann-Schwinger lite" in bound states (after Timofeyuk & Mukhamedzhanov; Pinkston & Satchler)

You can compute Schrödinger wave function accurately at small radius & extract asymptotic amplitudes with a "L-S" kernel (not exactly, but closely related)

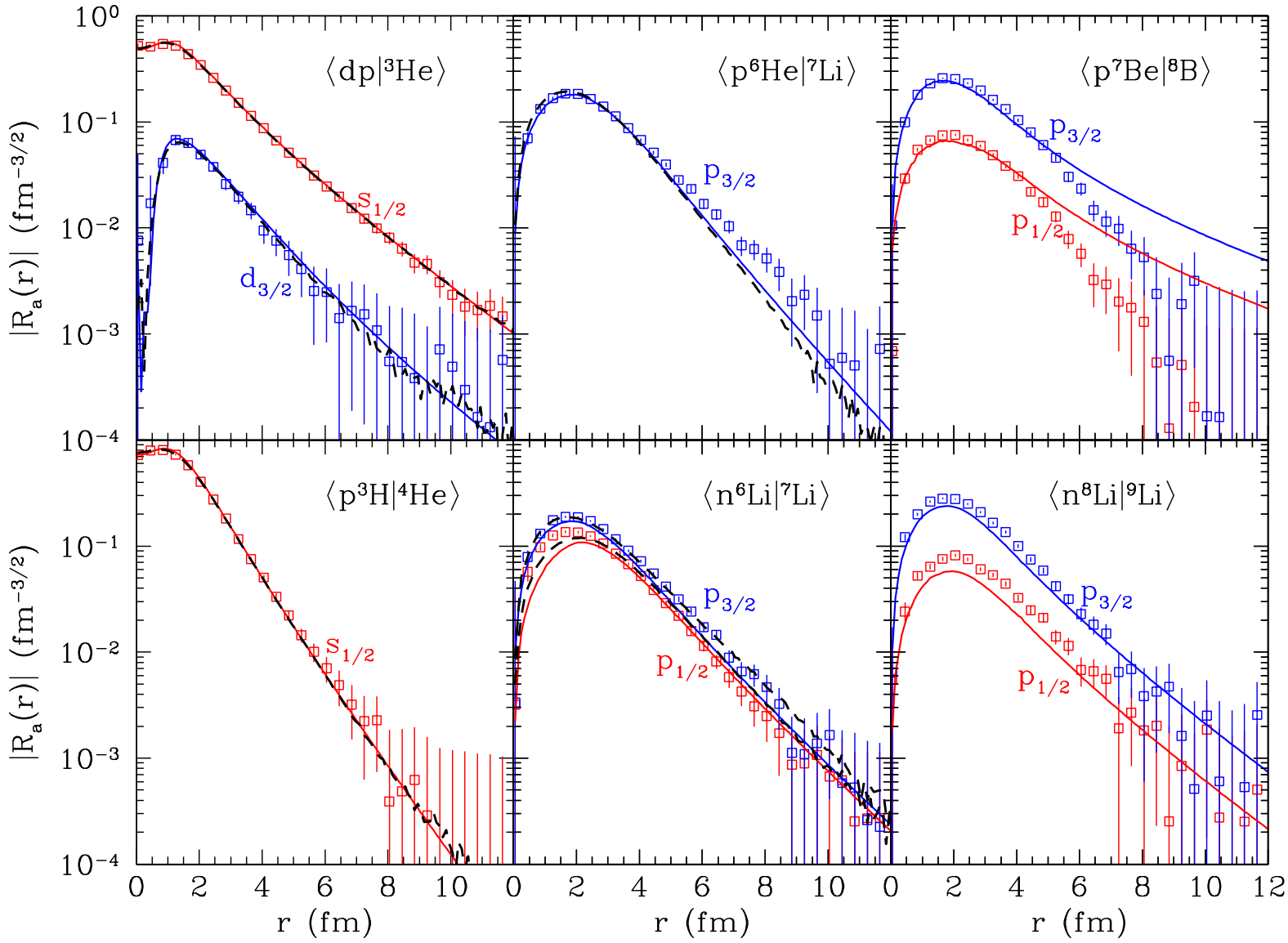
Actually works pretty well with variational Monte Carlo Ψ even without Green's function Monte Carlo

Asymptotic normalizations (ANCs) computed this way from VMC agree well with experiment

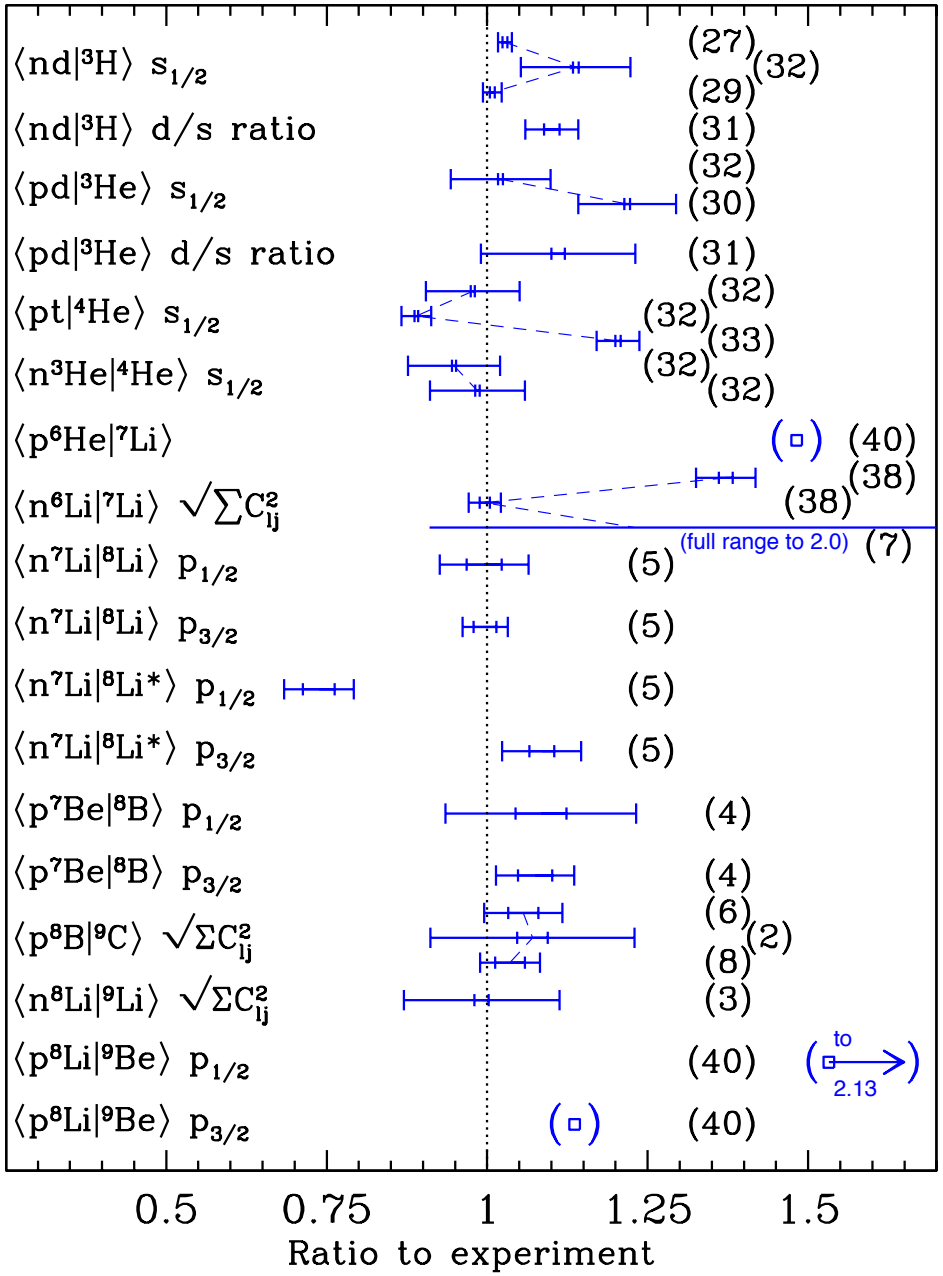
Cluster channel overlaps from VMC and L-S kernel

Points: Explicitly integrated Monte Carlo overlaps in VMC

Solid curves: Overlaps from VMC Ψ & L-S kernel



ANCs from VMC wave functions



THEORY DIVIDED BY DATA

Small error bars are VMC statistics

Large ones are “experimental”

Sensitivity to wave function construction seems weak but hard to quantify

$A \leq 4$ clearly dominated by systematics, also old

With a couple of exceptions, these are the first *ab initio* ANCs in $A > 4$

Unbound amplitudes: S-, K- or T-matrix

Scattering amplitudes are direct analogues of bound-state ANCs

There are two amplitudes (incoming/outgoing or regular/irregular) in each channel

$$\Psi \longrightarrow AF_l(kr)/r + BG_l(kr)/r$$

That's actually an advantage:

Observables depend on A/B, so Ψ error cancels at 1$^{\text{st}}$ order (Schwinger, Kohn variational principles)

For "particle-in-box" methods, the L-S kernel should extract accurate off-diagonal S-matrix elements from approximate Ψ

I have a student ramping up to application for coupled angular momentum channels in $^3\text{H} + n$ & $^3\text{He} + p$

Do we even want pure *ab initio* for astrophysics?

Ab initio reaction calculations probe NN & NNN interaction & computational methods

Eventually they should predict some cross sections better than phenomenology

BUT high precision even in moderate-A systems needs fine tuning
(e.g.: placement of thresholds is important)

Everyone doing *ab initio* capture reactions does some tuning for that
(e.g.: SRG evolution set up for correct threshold with no NNN)

Some maximally consistent way is needed to pull together complementary *ab initio* & empirical information

Halo EFT as a “fewer-body” framework

Halo effective field theory (EFT) can be used much like phenomenological R-matrix but might connect more simply to *ab initio* constraints

Instead of ordinary quantum mechanics, you take each nucleus as a particle in quantum field theory & develop a Lagrangian

You explicitly build in correct gauge, rotational, etc. symmetries

Lagrangian is expanded & truncated in terms of $(k/\Lambda)^n$, where Λ is breakdown scale (neglected threshold)

It’s “halo” EFT because it’s only useful for small binding energy – halo nuclei

Pursued by a few groups: Rupak & Higa; Hammer & Phillips; Ryberg, Forssén, Hammer & Platter

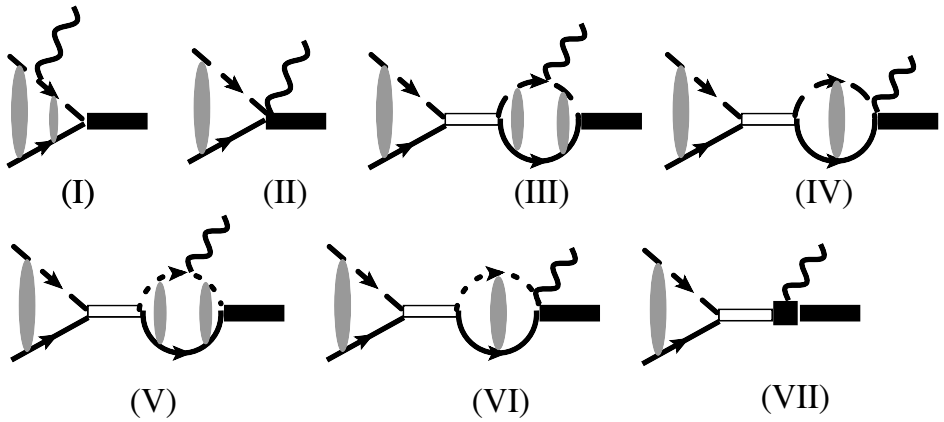
Halo EFT of $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$

Over a few papers, Xilin Zhang, Daniel Phillips & I developed an EFT of $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ at next-to-leading order (NLO) [cf. Ryberg et al., Rupak & Higa]

Key ingredients: Sum Coulomb at all orders & organize field theory renormalization in terms of physical parameters

The renormalized theory is in terms of ANCs, scattering lengths, effective ranges

$^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ S-factor calculation:



$$S(E) = f(E)\sum_s C_s^2 \Big[\; \big| \mathcal{S}_{\mathrm{EC}}\left(E;\delta_s(E)\right) + \overline{L}_s \mathcal{S}_{\mathrm{SD}}\left(E;\delta_s(E)\right) + \epsilon_s \mathcal{S}_{\mathrm{CX}}\left(E;\delta_s(E)\right) \big|^2 + |\mathcal{D}_{\mathrm{EC}}(E)|^2 \; \Big]$$

Halo EFT at next-to-leading order (NLO)

At NLO there are 9 parameters for $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$

2 ANCs: C_s $(s = 1, 2)$

2 short-distance couplings to the photon (like R-matrix internal capture): $\bar{L}_s$

1 coupling to excited ^{7}Be (essentially an ANC): ϵ_s

2-term effective-range expansion in each s-wave channel, modeled as an unbound "dimer" analogous to bound state: (a_s & r_s – yields phase shifts δ_S)

$$S(E) = f(E) \sum_s C_s^2 \Big[\Big| \mathcal{S}_{\mathsf{EC}}\left(E; \delta_s(E)\right) + \overline{L}_s \mathcal{S}_{\mathsf{SD}}\left(E; \delta_s(E)\right) + \epsilon_s \mathcal{S}_{\mathsf{CX}}\left(E; \delta_s(E)\right) \Big|^2 + |\mathcal{D}_{\mathsf{EC}}(E)|^2 \Big]$$

The $\mathcal{S}$ & $\mathcal{D}$ matrix elements are very close to parts of Barker & Kajino R-matrix

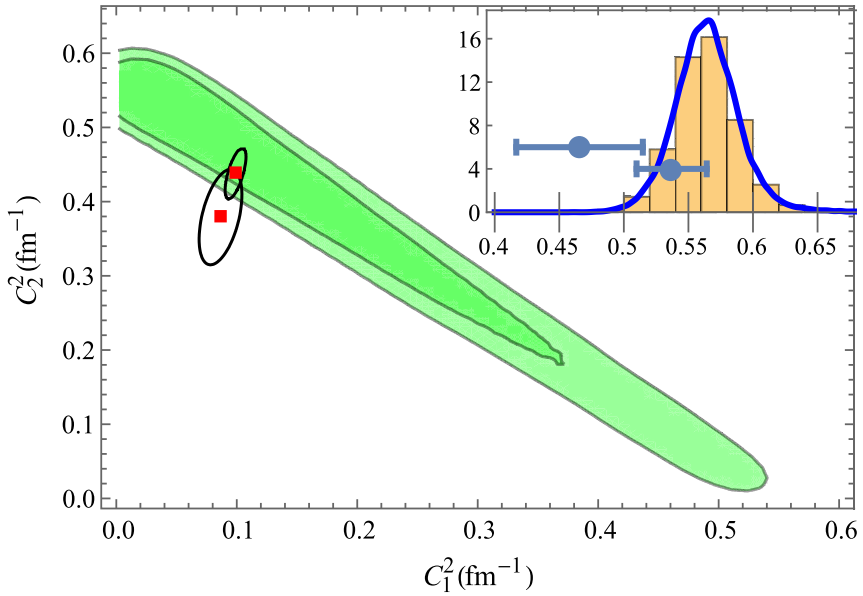
Bayesian treatment of parameters

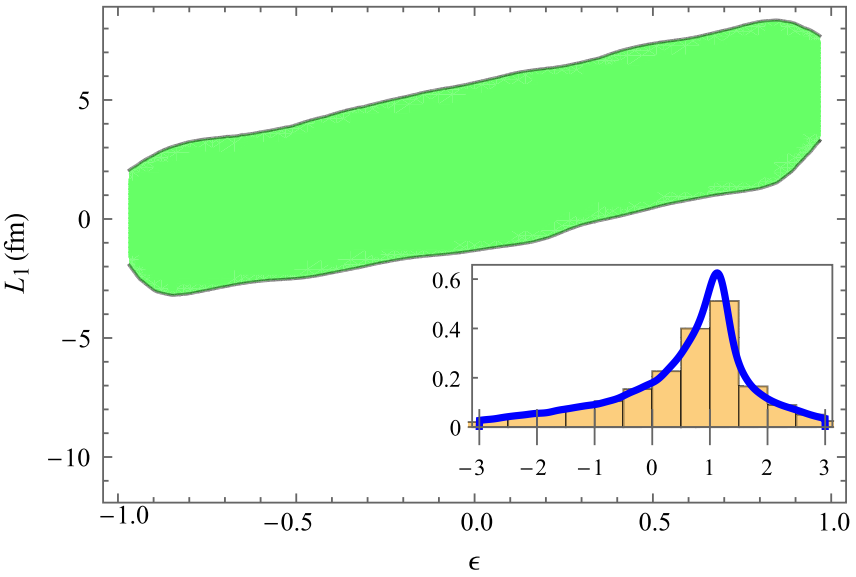
None of the 9 parameters are well-determined by data, but $S(E < 500$ keV) is

We computed Bayesian posterior probability of $S(E)$ from capture data, with scattering lengths & floating norms as Gaussian-distributed priors

We fitted at $E < 500$ keV to avoid resonances $\longrightarrow (k/\Lambda)^2 \lesssim 4\%$ estimates truncation error conservatively (marginalizes out to 0.2% on $S(0)$)

We also tried experiment & *ab initio* ANC priors, but eventually left them out





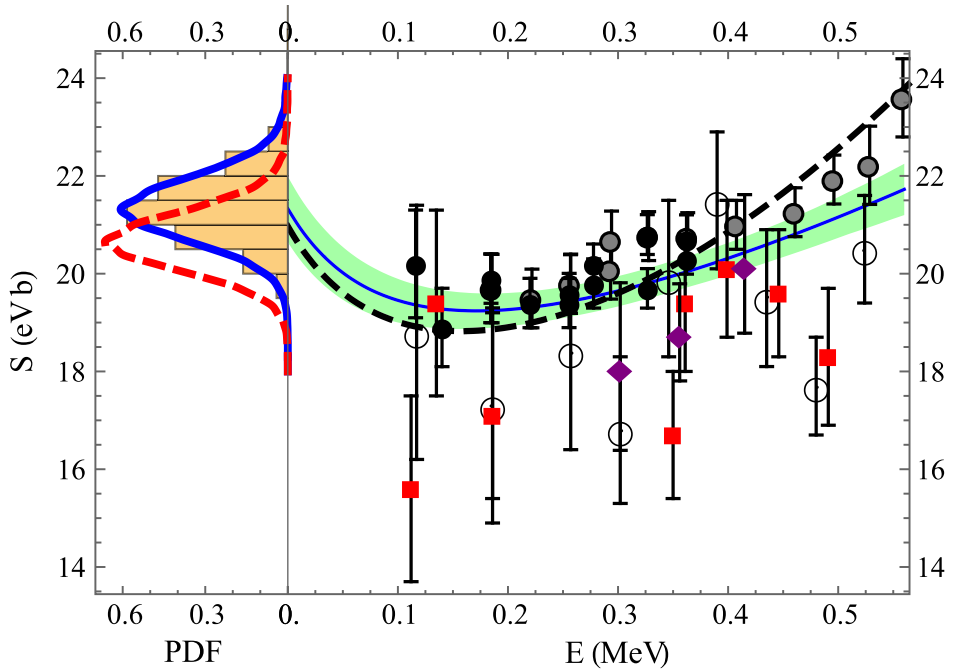
Zhang, Nollett, Phillips, PLB **751**, 535 (2015)

What we really want for $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ is $S(0)$ or $S(20\ \mathrm{keV})$

Marginalizing over all parameters, we find $S(0) = 21.3 \pm 0.7$ eV b

Solar Fusion II recommends $S(0) = 20.8 \pm 0.7\,(\mathrm{ex}) \pm 1.4\,(\mathrm{th})$ eV b

Navrátil et al. compute $S(0) = 19.4 \pm 0.7$ eV b *ab initio*, error from truncation



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Full histogram: $S(0)$

Dashed histogram: $S(20\ \mathrm{keV})$

Green band: Marginalized $S(E)$

Solid curve: Parameters matching band median

Dashed curve: Keeping only LO parameters from solid curve

Some thoughts on the future

^{7}Be$(p,\gamma)^8$B experience suggests a path toward smart use of *ab initio* information:

Construct a "fewer-body" model like R-matrix, Woods-Saxon, or halo EFT

Compute some of its parameters *ab initio* & use those and e.g. threshold energies as Bayesian priors

Then use MCMC to estimate the extrapolated cross section you care about from reaction data

Ab initio methods should eventually provide priors on more parameters than just ANCs

Down the road a bit

Lippmann-Schwinger & similar techniques may provide a natural path that links *ab initio* calculations consistently with multiple EFT parameters

Even purely *ab initio* models will be more efficient & useful if they can produce *honest* parameters for fewer-body halo EFT, R-matrix, or potential models

By "honest," I mean no hand-waving, actually one-to-one between the models

Specifically for halo EFT:

We're working on Bayesian $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ now – nearly same structure, different data & separation energies [differently-organized EFT by Higa et al.]

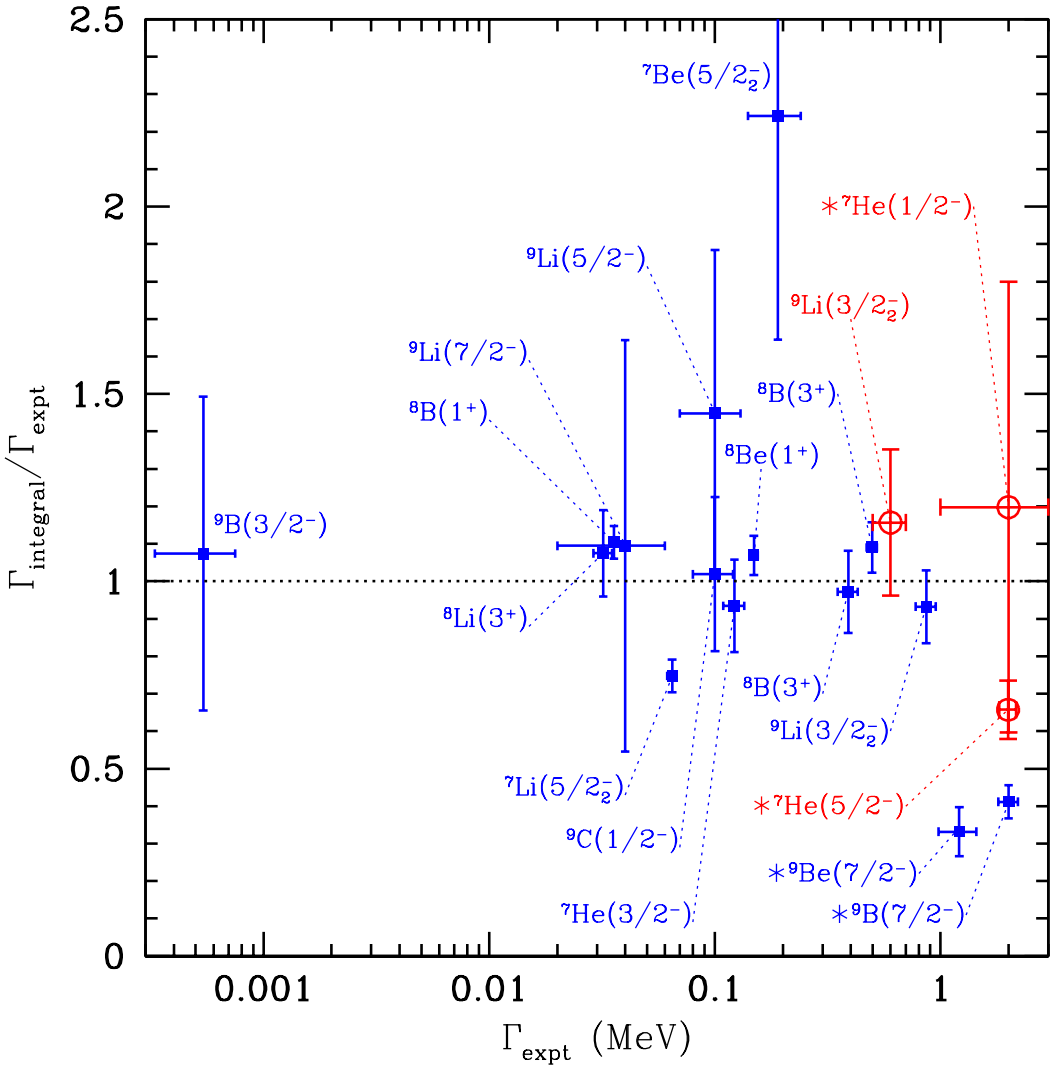
At least for setting priors, we need a better approach to Pauli-principle constraints that impose nodes on channel overlaps

BONUS MATERIAL

Testing out the L-S estimates of Γ

The integral estimate should apply to states that are in some sense narrow

I've chosen low-lying states in $A \leq 9$ with mainly/purely nucleon decays



Red: overlaps inconsistent with resonance

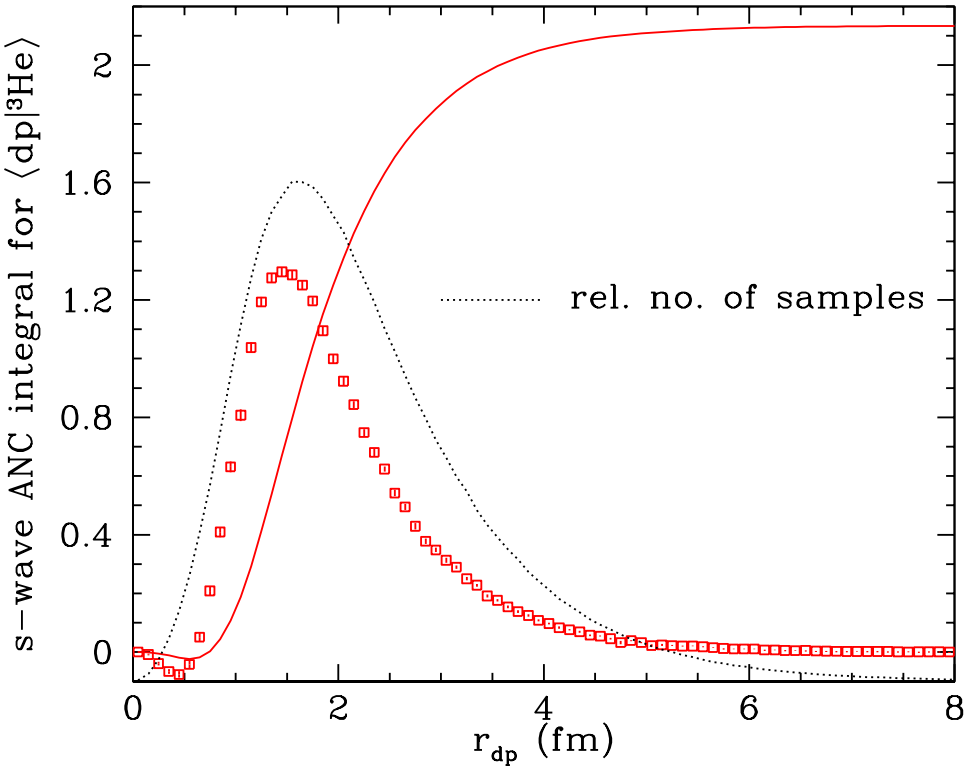
Asterisk: uncomputed channels

Dynamic range of 0.0005 to $\lesssim$ 1.0 MeV, not otherwise possible for QMC

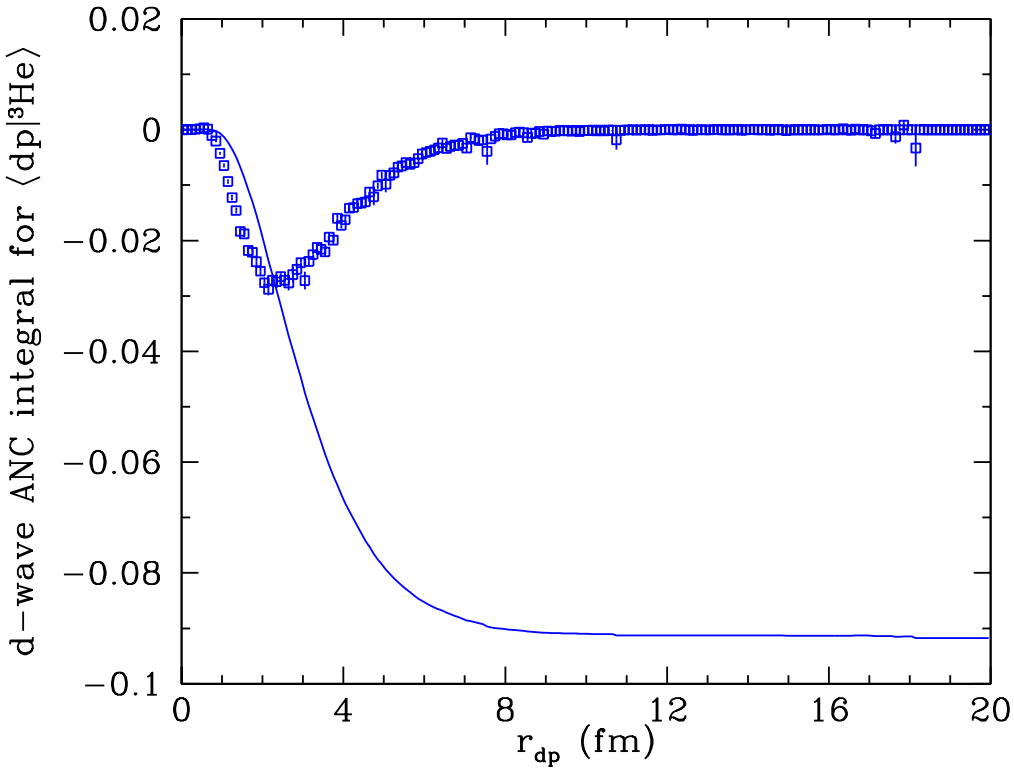
Turned out about as accurate as it has any right to be

Short range of the kernel: ^{3}He $\rightarrow$ dp asymptotic normalizations (ANCs)

s-wave ANC integrand & integral



d-wave ANC integrand & integral



Points are Monte-Carlo sampled integrand; solid curves are cumulative integrals

For ^{3}He $\rightarrow$ dp, we have $C_s^{dp} = 2.131(8)$ fm$^{-1/2}$, $C_d^{dp} = -0.0885(7)$ fm$^{-1/2}$

ANCs converge just where sampling gets sparse in the explicit overlap