Quantum Monte Carlo calculations of reaction and scattering processes

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The variational Monte Carlo method (even useful by itself)

Variational Monte Carlo (VMC) is built on a sophisticated Ansatz for the wave function, built on shell-model-like structure modified by operator correlations:

$$\Psi_T = \text{[3-body operator functions]} \times \text{[2-body operator functions]} \times \text{[scalar functions]} \times \text{[shell-model-like orbital/spin/isospin structure]}$$

Two-body correlations solve sets of differential equations built on the potential, three-body based on 1$^{\text{st}}$-order perturbation

Each piece contains adjustable parameters

We evaluate $E_T = \dfrac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$, a variational bound on ground state energy for given J^π and isospin

We change the parameters by hand, re-compute E_T, and minimize E_T to obtain improving approximations to the ground state and its energy

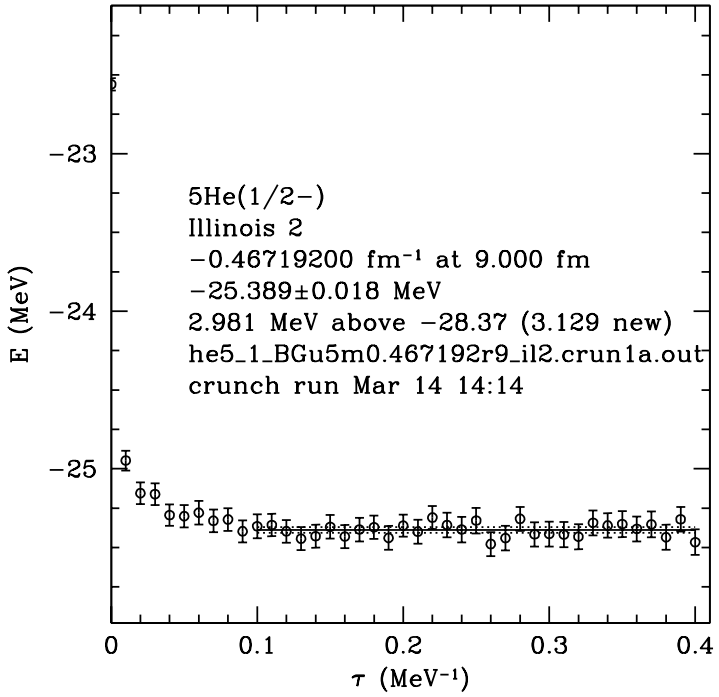
Green's function Monte Carlo

Green's function Monte Carlo (GFMC) is an operator method that projects the true ground state out of the VMC wave function

$$\Psi(\tau) = \exp\left[-\left(H - \tilde{E}\right)\tau\right]\Psi_T$$

As $\tau \to \infty$, $\Psi(\tau)$ approaches the ground state

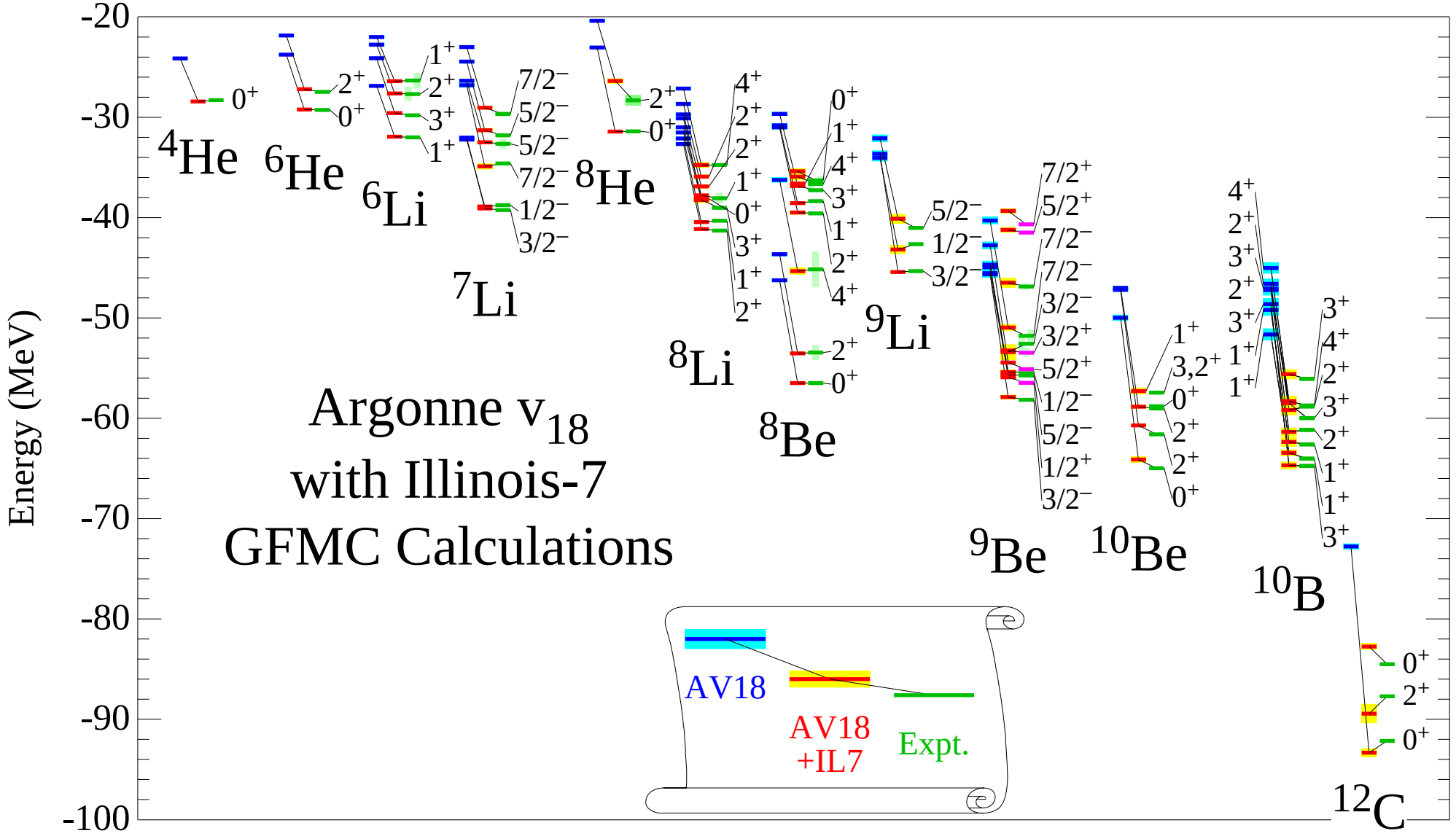
The operator $\exp\left[-\left(H - \tilde{E}\right)\Delta\tau\right]$ is written as an integral over a Green's function



Integration is by Monte Carlo, sending many samples of Ψ_T on random walks through particle configurations (with path constraint)

We have examined many bound and narrow states using this method

Energies of broad states (100s of keV) do not converge



From a very thorough review by Carlson et al. at arXiv:1412.3081

Quantum Monte Carlo: Il buono

Our main advantage & disadvantage is that there is no expansion in spatial basis functions*

We can incorporate hard-core interactions & long-range asymptotics relatively easily (not always as precisely as we'd like)

We can in principle compute anything on the real E axis (not poles)

NNN force terms are computationally tractable in at least the lower p-shell

Quantum Monte Carlo: Il Cattivo e/o Brutto

We're in trouble if we run into a case where we can't make a good variational guess (intruder states?)

We only get one state at a time, not several states from Lanczos diagonalization

We need a local or nearly-local Hamiltonian for GFMC, though this has recently come under control for chiral interactions

GFMC/VMC calculations grow rapidly with A, so they may not go past $A = 12$

Auxiliary field diffusion Monte Carlo (AFDMC) can handle larger systems, but has its own limitations

Beyond bound & narrow: A quantum Monte Carlo approach to scattering

Quantum Monte Carlo methods are (mostly) variational – they produce the lowest energy level satisfying the imposed constraints

Most direct application to scattering requires setting it up as an eigenvalue problem with discrete states

Past applications (nuclear, atomic, solid state) have been "particle in a box" with wave function constrained to zero at the box surface $r_{12} = R_0$

After energy is computed, match onto

$$\Psi \propto \frac{1}{kr_{12}} \{\Phi_{c1}\Phi_{c2}Y_L\}_J \left[\cos\delta_{JL} F_L(kr_{12}) + \sin\delta_{JL} G_L(kr_{12})\right] \ ,$$

so $\tan\delta_{JL} = -F_L(kR_0)/G_L(kR_0)$

Improving on the nodal boundary condition

There are drawbacks to the nodal boundary condition, the worst being that low energy $\longrightarrow$ an enormous box (long de Broglie wavelength)

An R-matrix boundary condition is better:

$$\hat{\mathbf{n}} \cdot \nabla_{\mathbf{r}} \Psi = \gamma \Psi \ , \quad \text{at } r = R_0$$

We can then fix R_0 at some "small" value (beyond nuclear interaction and nucleon exchanges)

γ is specified by construction in VMC or method of images in GFMC

We choose several γ to get states of different $E(\gamma)$, match at surface to get $\delta(E)$

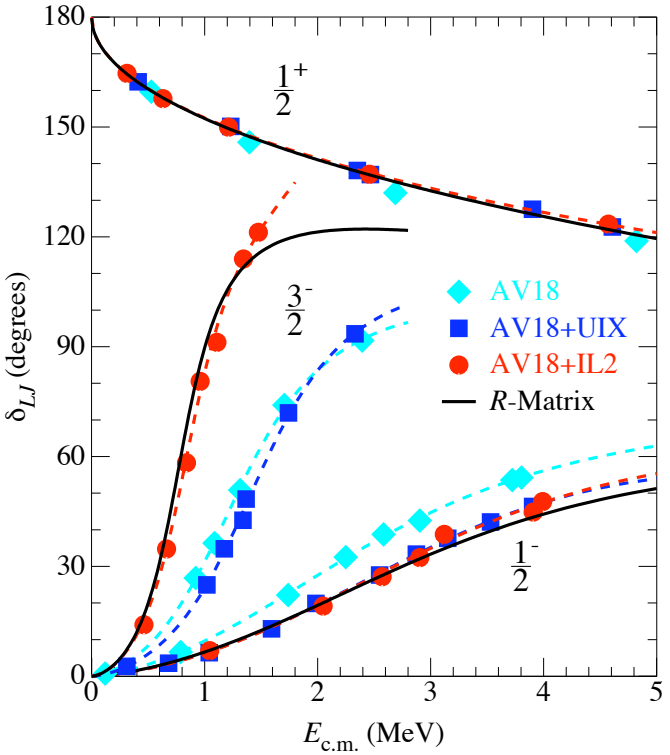
Generalizable to multiple open channels or higher energy with excited-state methods (but not yet)

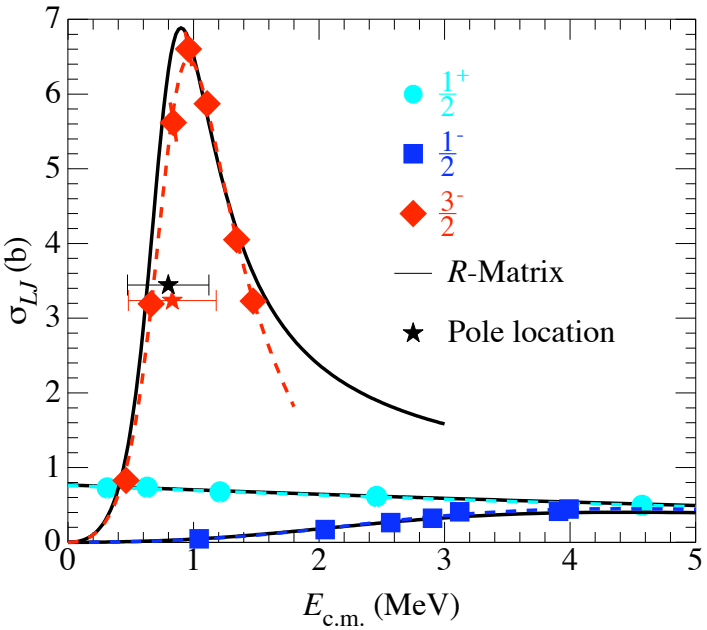
First exercise: $^4\mathrm{He} + n$

s-waves turn out similarly for all interactions

Scattering lengths all consistent with 2.4 fm,
compared with 2.46 fm measured

	$3/2^-$ (MeV)	$1/2^-$ (MeV)
Argonne v_{18}	$1.19 - 0.77i$	$1.7 - 2.2i$
AV18+UIX	$1.39 - 0.75i$	$2.4 - 2.5i$
AV18+IL2	$0.83 - 0.35i$	$2.3 - 2.6i$
Experiment	$0.798 - 0.324i$	$2.07 - 2.79i$





The numbers produced can also be compared directly with cross sections

Alternatively, locations of poles off real axis have to be fitted as you would do with experimental data

All described in PRL 99, 022502 (2007)

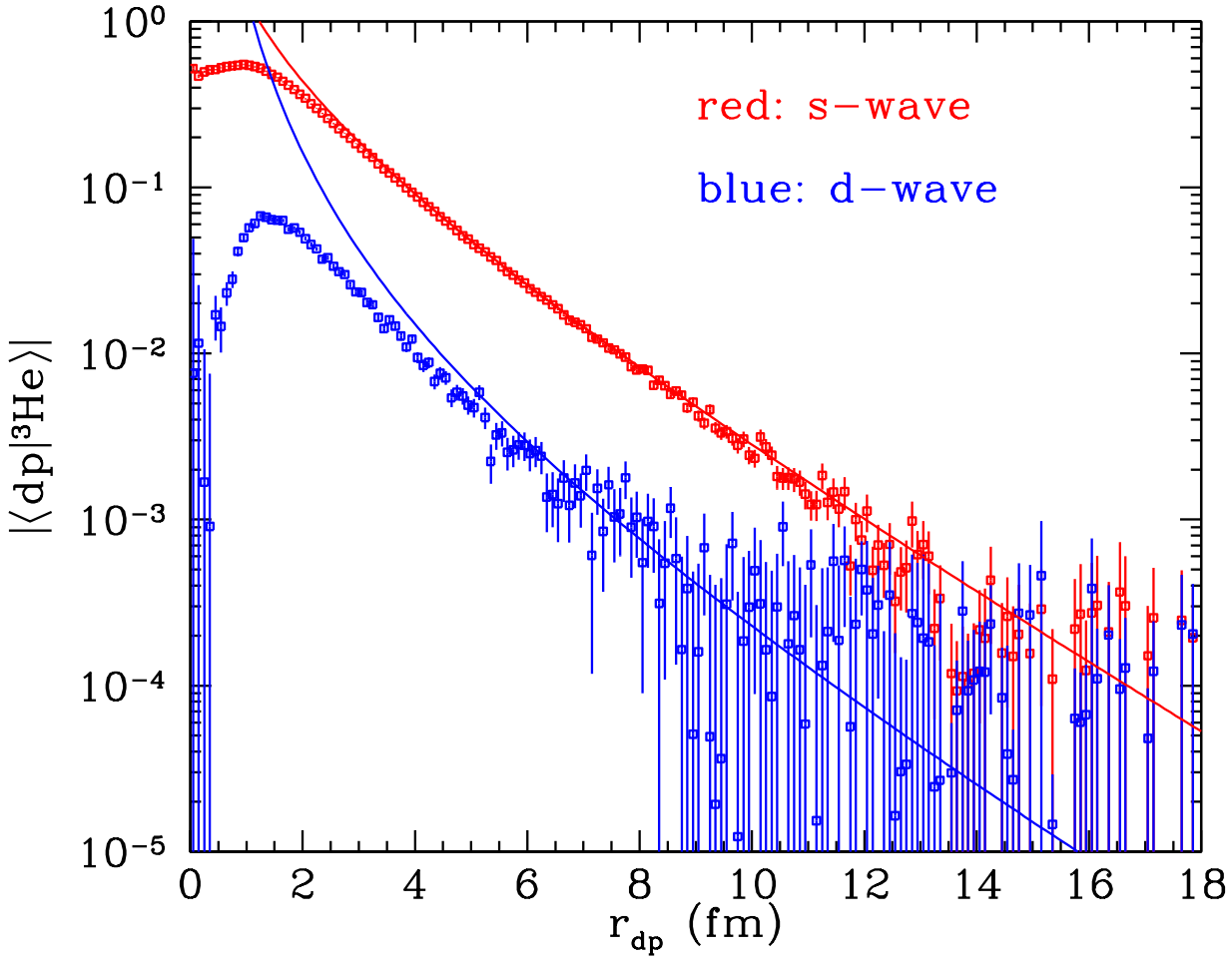
Next steps for scattering

Things I would like to do or see done soon in QMC are:

- compute ^{5}He parity violation (n spin rotation in ^{4}He)
- complete $p\,^3$He & $n\,^3$H scattering calculations with GFMC
- unbound states previously treated as bound ("successfully" and not)
- resonant (and not) $\alpha\alpha$ scattering and ^{8}Be states
- continued learning on coupled channels, e.g. $n+\,^3$He, $p+\,^3$H, $d+d$
- electroweak captures with GFMC, including exchange current & relativistic terms
- chiral potentials, not just AV18+UIX/IL7

Asymptotic normalization coefficients (ANCs)

At large cluster separations, correlations within nuclei have known shapes from Schrödinger Eq. with at most Coulomb term



The many-body dynamics give the separation energy (hence η & k), and normalization of $CW_{-\eta,l+1/2}(2kr)/r$ or $C\sqrt{k/\pi r}K_{l+1/2}(kr)$

Asymptotic normalization coefficients (ANCs)

ANCs characterize the nuclear surface & can dominate some transfer or radiative-capture reactions

ANCs are closely related to particle widths, at least for narrow states, because $-E \longrightarrow +E$ takes $W \longrightarrow G + iF$,

Extraction of outer parts of overlaps from QMC wave functions can be problematic

Good Monte Carlo sampling in the tails is tough, especially for small components

Putting correct asymptotics into Ψ_T without breaking something else can be difficult – trouble for many observables, including ANCs

But can we get correct asymptotics out of VMC without putting it in?

Integral relation for the ANC

Yes – we can learn the ANC from an approximate wave function with a bad tail (goes back to 1970s)

The Schrödinger equation

$$(H - E)\,\Psi_A = 0$$

may be separated into parts internal to Ψ_{A-1} and parts involving the last particle (distance r_{cc} away) to yield

$$\Psi_A \;=\; -\left[T_{\rm rel} + V_C + B\right]^{-1}\left(U_{\rm rel} - V_C\right)\Psi_A$$

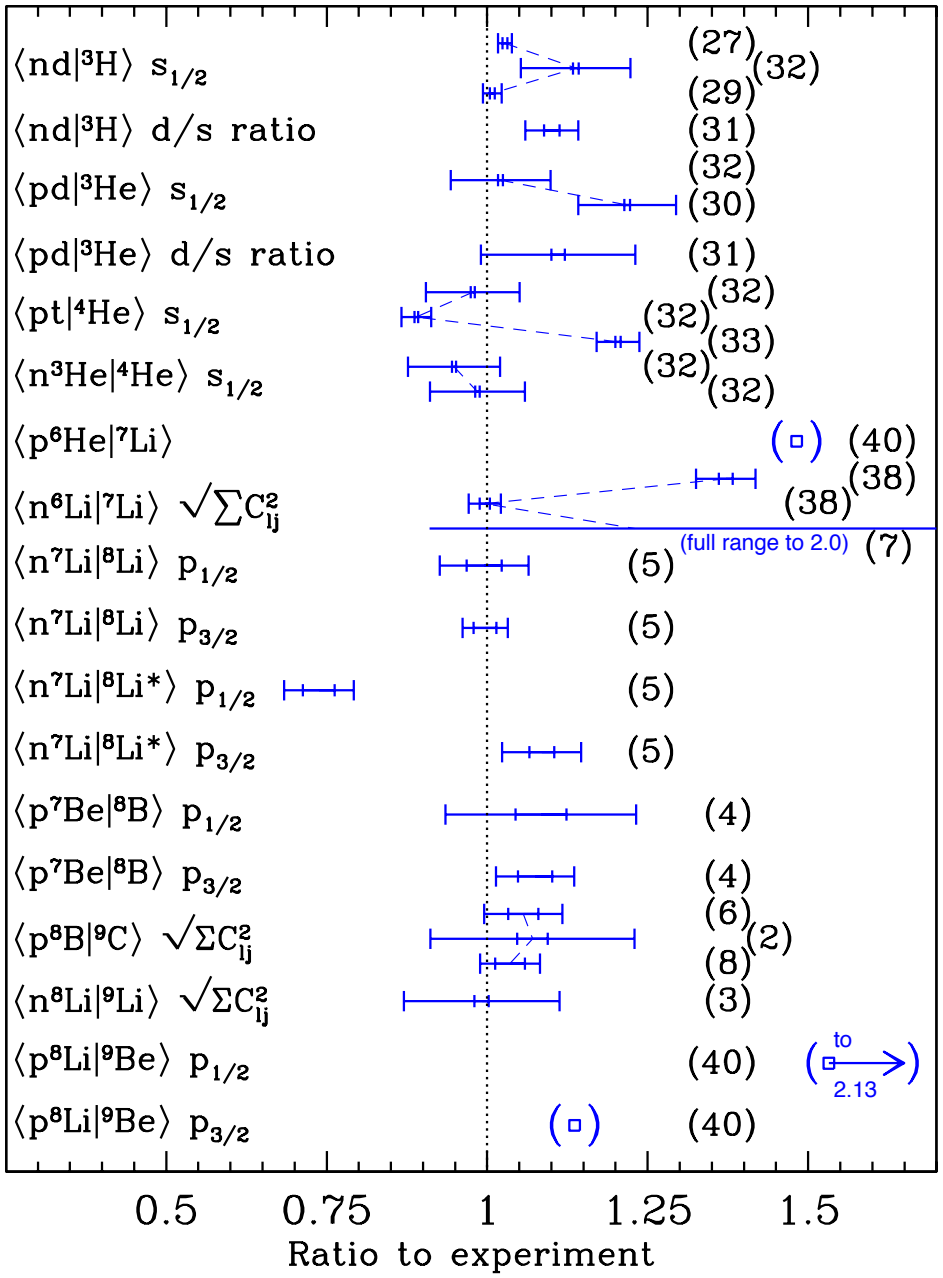
which implies

$$C_{lj} = \frac{2\mu}{k\hbar^2 w}\mathcal{A}\int \frac{M_{-\eta,l+\frac{1}{2}}(2kr_{cc})}{r_{cc}}\Psi^\dagger_{A-1}\chi^\dagger Y^\dagger_{lm}(\hat{\mathbf{r}}_{cc})\left(U_{\rm rel} - V_C\right)\Psi_A d\mathbf{R}$$

$M_{-\eta,l+\frac{1}{2}}(2kr)$ is the "other" Whittaker function, irregular at $r \to \infty$,

and $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_A)$, with $r_{cc} = \mathbf{r}_A - \frac{1}{A-1}\sum_{i=1}^{A-1}\mathbf{r}_i$

ANCs from VMC wave functions



Small error bars are VMC statistics
This isn't GFMC

Large ones are "experimental"

Sensitivity to wave function construction seems weak but hard to quantify

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

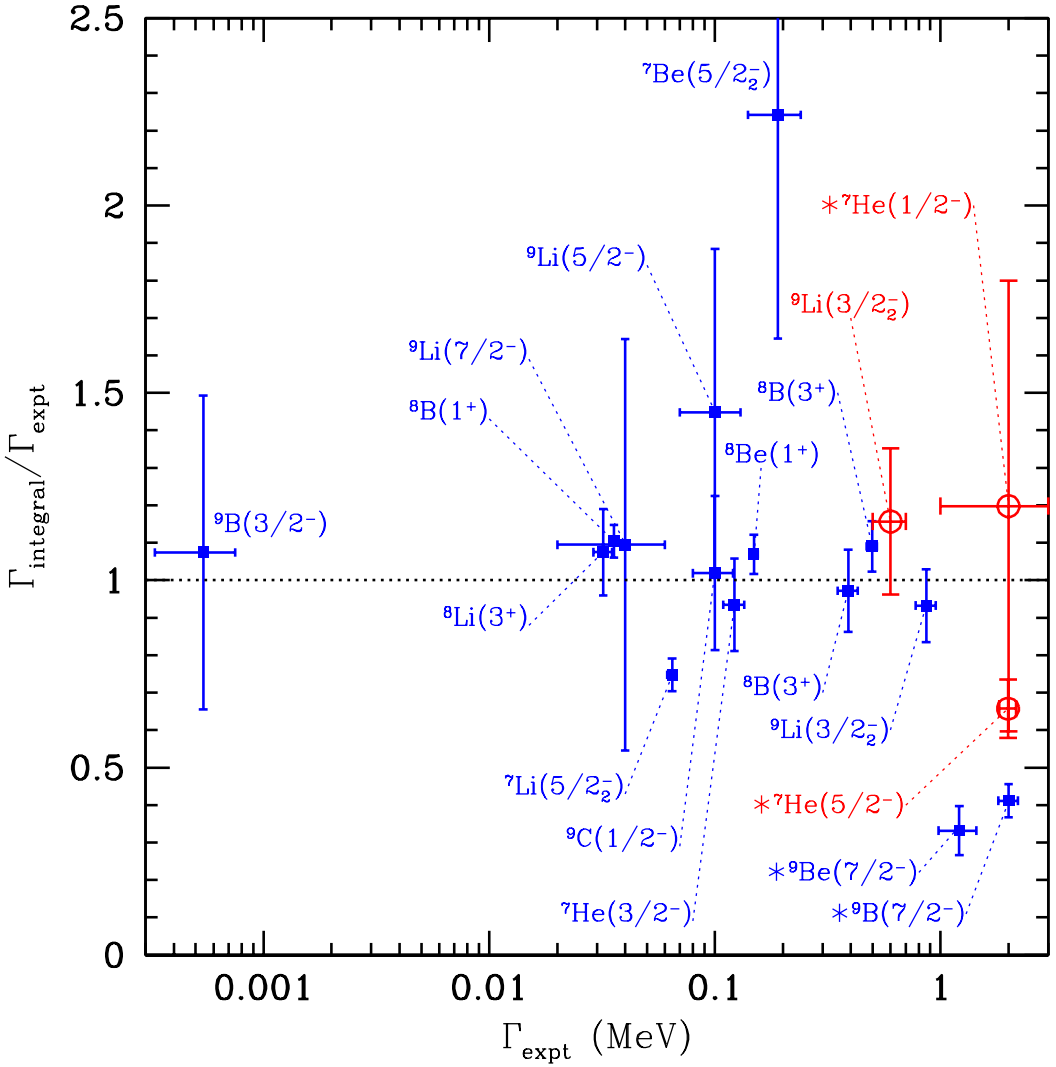
With a couple of exceptions, these are the first *ab initio* ANCs in $A > 4$

Good agreement emerged once experimental separation energies were put into the calculation

Widths as squared ANCs of resonant states

Widths are proportional to ANCs of resonant states, $\Gamma \simeq \frac{\hbar^2 k}{\mu}|C_{lj}|^2$

I've chosen low-lying states in $A \leq 9$ with width mainly/all in nucleon emission



Red: overlaps inconsistent with resonance

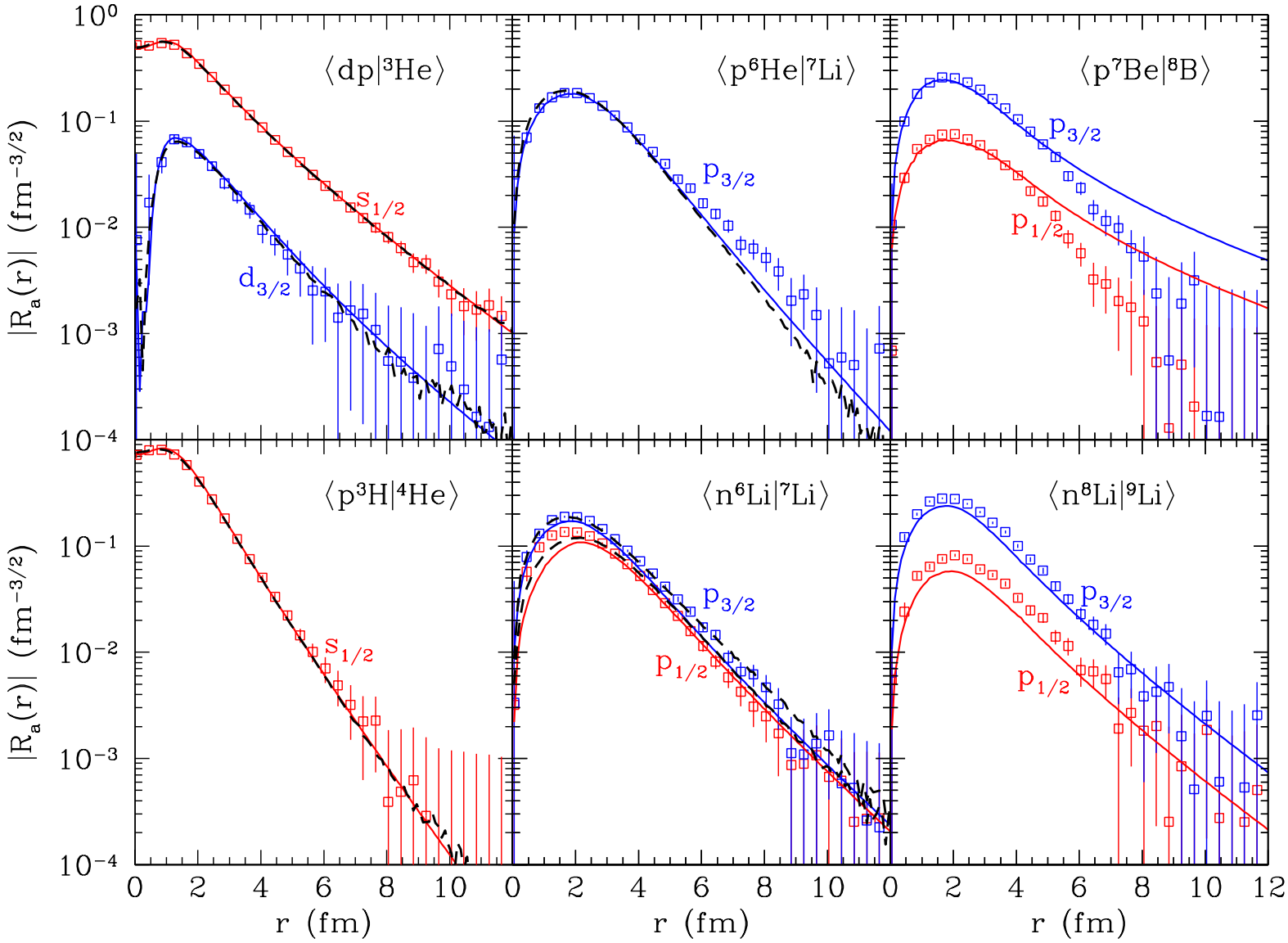
Asterisk: uncomputed channels

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

Nollett, PRC 86, 044330 (2012)
Nollett & Wiringa, PRC 83, 041001 (2011)

Overlaps at all radii: not just asymptotics

The integral relations contain more information about the potential than does the VMC wave function $\longrightarrow$ better overlaps



What next?

α (& other cluster) widths & overlaps once the code is more-generally written

Tests against scattering calculations

GFMC and IL7 (better match to experimental thresholds)

Similar things are being done as pseudobound approaches to scattering $\delta(E)$ (Horiuchi et al., Kievsky et al., etc.) – some of that can be adapted

Coupled-channel problems will require some way of extracting surface amplitudes from GFMC, integrals are probably the way to do that

GFMC has trouble resolving $\Delta E \lesssim 100$ keV, so integral relations on pseudobound states will beat particle-in-a-box for widths of narrow states

A way to generate small parity impurities from P violating Hamiltonian terms?

Encapsulating *ab initio* information in ANCs (& similar operators?)

Important information in an *ab initio* model can often be represented as parameters of a simpler model

You can get a long way with separation energies, scattering lengths, widths and/or ANCs

This underlies the claims to measure ANCs in transfer reactions using non-*ab initio* reaction theory

You can also set up a reasonably good direct capture model with a separation energy, a scattering length or two, & some ANCs

Again, this depends a little on your goals & what precision you want

Ab initio ANCs in an EFT

Xilin Zhang incorporated my computed ANCs into halo EFT models of $^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$ & $^{7}\mathrm{Li}(n,\gamma)^{8}\mathrm{Li}$

The captured nucleon & target nucleus are set up as fundamental fields

The Langrangian is a power series expansion in a ratio of momentum scales (separation momentum over core-excitation momentum)

Xilin has nice results at leading order – inputs are scattering lengths, separation energies & ANCs

At next-to-leading order there are more parameters, but ignorance of them appears unimportant for capture at threshold

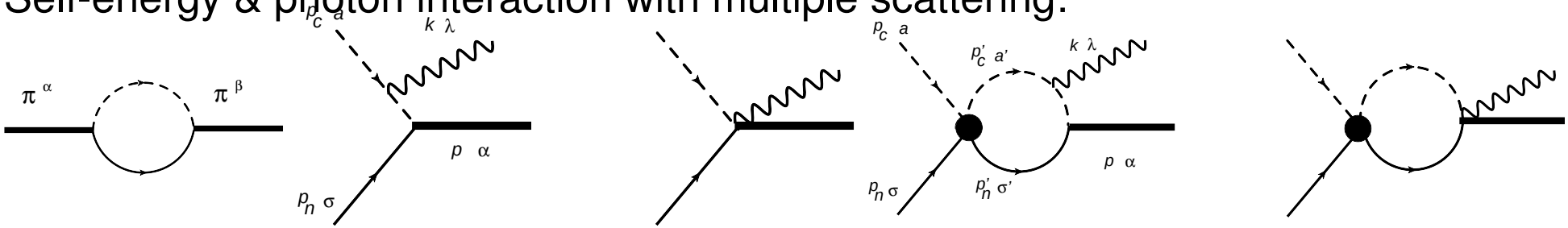
Halo EFT

For ^{7}Li$(n,\gamma)^8$Li, we have fields for ^{7}Li, ^{7}Li*, n, ^{8}Li(2^+), & ^{8}Li(1^+)

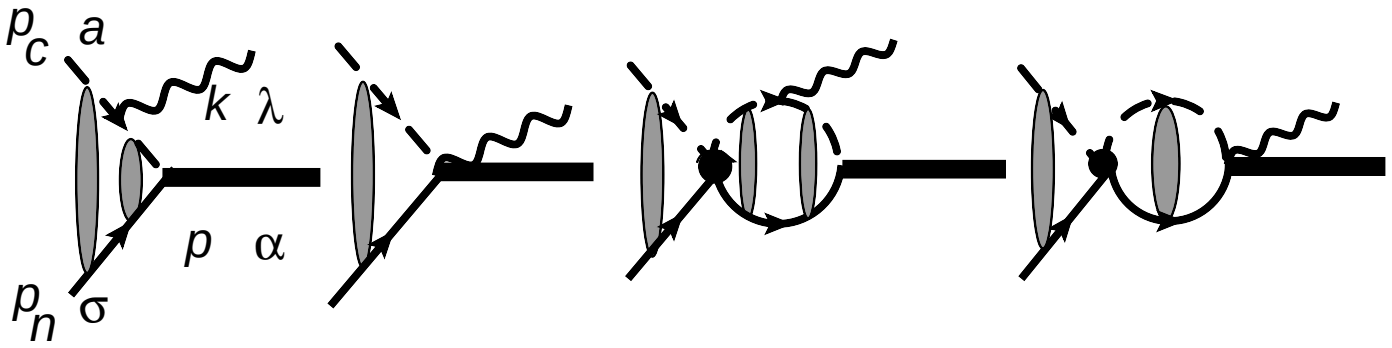
Our Lagrangian has kinetic and coupling terms, and interaction with photons

ANC fixes p-wave neutron-core-^{8}Li coupling, scattering lengths fix s-wave couplings

Self-energy & photon interaction with multiple scattering:



^{8}B is analogous, but we need to include multiple scattering with Coulomb included, at all orders

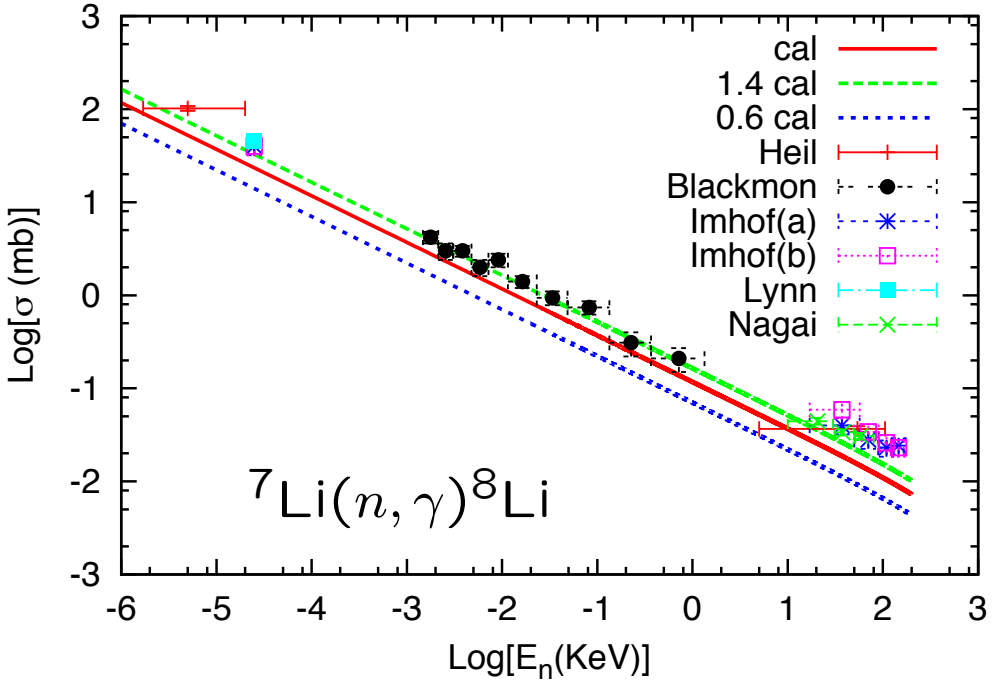


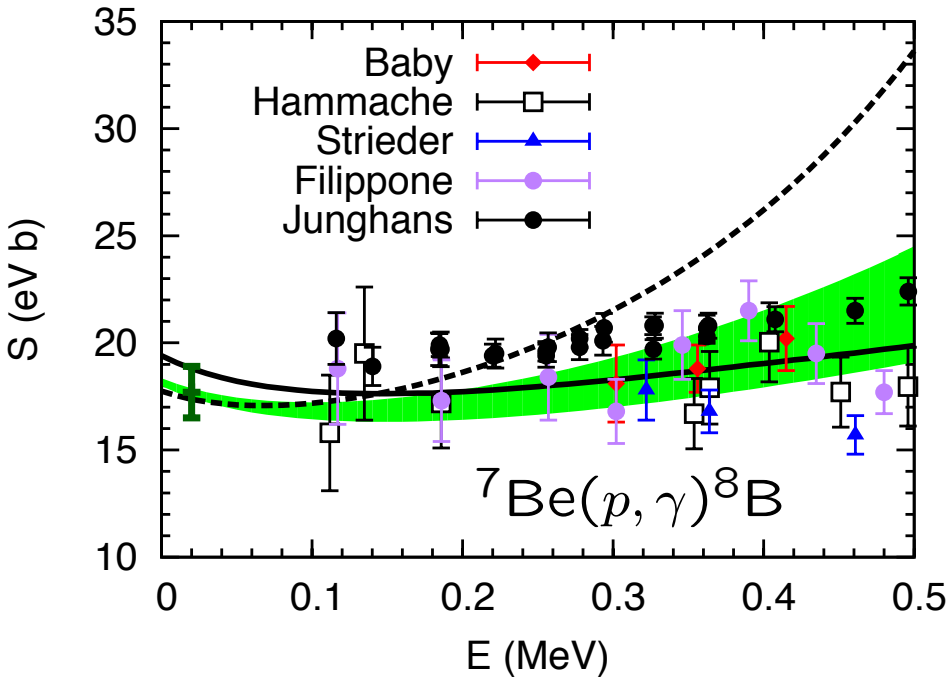
EFT+QMC results

Keeping in mind that these are leading-order calculations with 20–40% errors, the published results are not bad

For $^7\mathrm{Li}(n,\gamma)^8\mathrm{Li}$ we reproduce branching ratios amazingly well

For $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$ we agree with low-energy data, but there are fewer measured observables (^{7}Be & ^{8}B are both radioactive)





Zhang, Nollett, Phillips, PRC 89, 024613 (2014); 89, 051602 (2014)

Eclectic or fewer-body models

Incorporating *ab initio* information in leading-order halo EFT already seems useful for particular observables at the 5% level

The hope (under investigation) is that in next order – or other systems – there will continue to be couplings expressible as *ab initio* operators

It's important to do end-to-end *ab initio* calculations of cross sections, but they won't always be the best use of *ab initio* techniques

For applications, a completely *ab initio* model without adjustable parameters may be too good

For solar or big bang rates, we need something we can combine with data or use in some way to weight data, not something that stands apart

A "fewer body" model with some *ab initio* & some schematic/empirical pieces will be required or just more efficient sometimes