The outer limits of quantum Monte Carlo calculations

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For the next hour sit quietly, and we will control what you see and hear...

You've heard a few talks about *ab initio* nuclear calculations, so here's my quick summary of the program:

See how much of nuclear physics can be described accurately by neutrons & protons with vacuum interactions

Develop the interactions & currents to provide that accurate description

Provide a predictive tool for nuclear structure and reactions (e.g. for astrophysics)

Nuclear physics in a Mediterranean climate

Distinctive features of quantum Monte Carlo calculations relative to others

Lower storage & processing demands (at least to $A \leq 12$)

No particular need for a soft core, a weak three-body interaction, or renormalization to achieve those things

Keep the need for effective currents, quenching, etc. to a minimum

Intruder states no more demanding than natural parity

Straightforward extension to many unbound and other strong-clustering problems (no basis)

Potentials I

We work with the Argonne v_{18} nucleon-nucleon potential

It's one of several realistic potentials on the market

- fits all pp & np data to 350 MeV in Nijmegen 1993 phase shift analysis with $\chi^2_\nu = 1.09$, also deuteron binding energy
- 18 operator terms ($\mathbf{L}\cdot\mathbf{S}$, $\sigma\cdot\sigma$, tensor, scalar...), $\sim$40 parameters fitted once fifteen years ago
- local interaction, strong repulsive core, strong tensor interaction and π exchange at longer range
- full complication of EM interaction (mag. moment, vacuum polarization...), charge symmetry breaking, charge dependence

Potentials II

In $A \geq 3$ systems, there is an important 3-nucleon interaction that provides a large fraction of the binding energy & spin-orbit splitting

We use (mostly) the Illinois NNN interactions:

- 4 terms, spatial/spin/isospin dependence fixed by 2- & 3-pion exchange
- only 4 adjusted parameters (strengths of those terms)
- fixed by fit to ~ 20 bound and narrow levels at $A \leq 8$
- IL7 RMS deviation of 600 keV from 60 experimental states in $A \leq 10$

Illinois-7 is most recent re-fit, bug fix and added repulsion in $T = 3/2$ triples

The variational Monte Carlo method

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

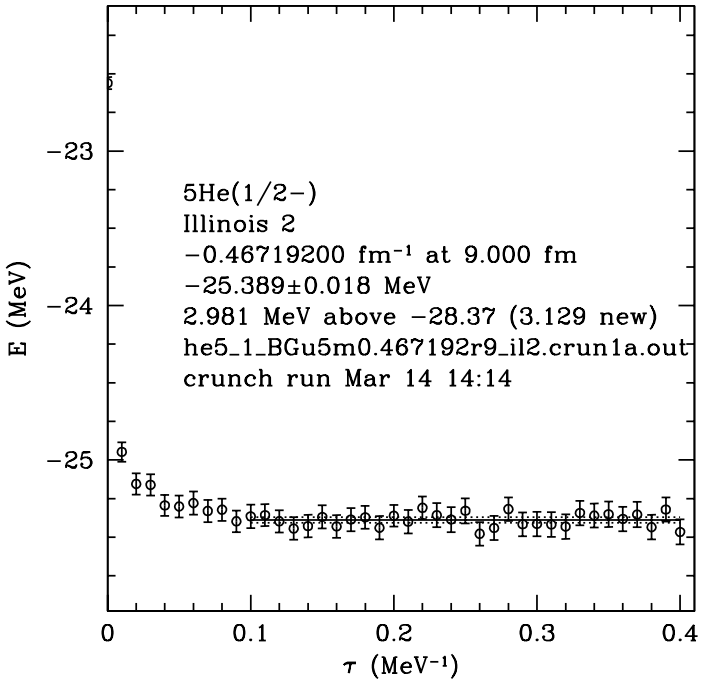
Green's function Monte Carlo I

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

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

Ψ_T comes from VMC – a good guess is vital to fast convergence

As $\tau \longrightarrow \infty$, $\Psi(\tau)$ 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 computed by Monte Carlo integration

Integration is done by generating many samples of Ψ_T and sending each on a random walk through particle configurations

Green's function Monte Carlo II

We impose a path constraint to mitigate the fermion sign problem

Final $\Psi(\tau)$ is sampled at discrete points in the particle coordinates

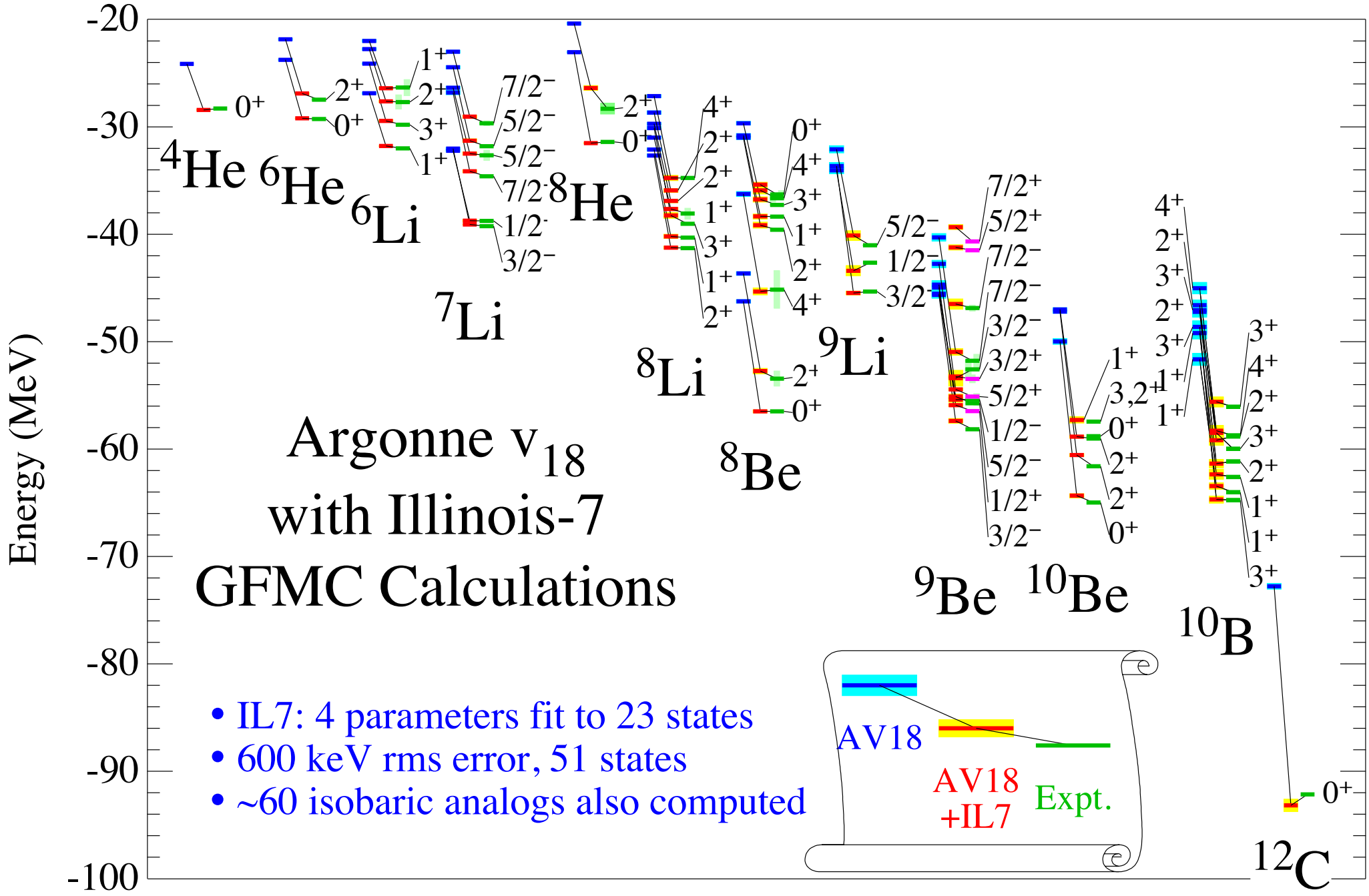
Expectation values are approximated by $\langle \Psi_T | \mathcal{O} | \Psi(\tau) \rangle$ and corrected perturbatively to obtain $\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle$

Not the case with $\langle H \rangle$ since H commutes with $\exp\left[-\left(H - \tilde{E}\right)\tau\right]$

We have examined many bound and narrow states using this method

Energies of broad states do not converge

No way has been found to obtain widths or good estimates of error introduced by pseudo-bound treatment of unbound states

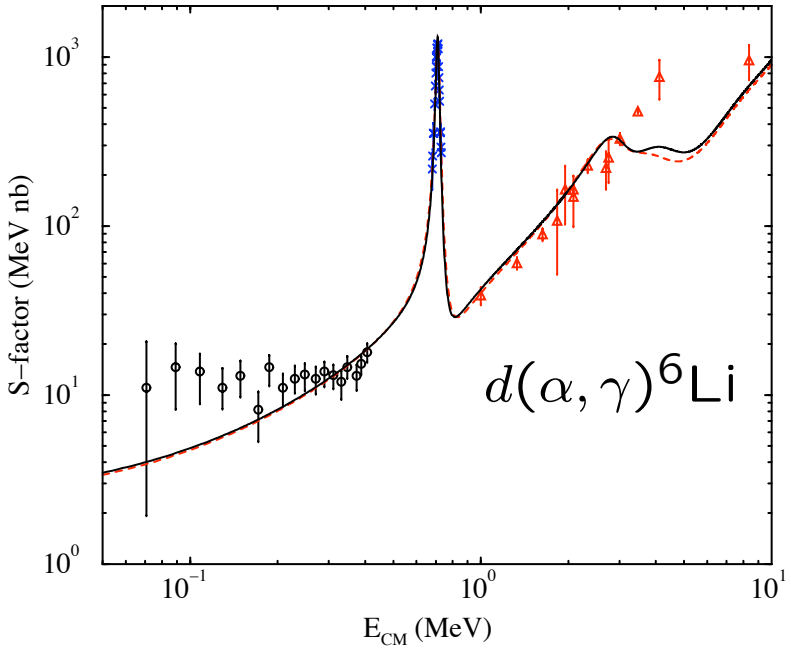

Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C
Argonne v18
with Illinois-7
GFMC Calculations
• IL7: 4 parameters fit to 23 states
• 600 keV rms error, 51 states
• ~60 isobaric analogs also computed
AV18
AV18
+IL7
Expt.

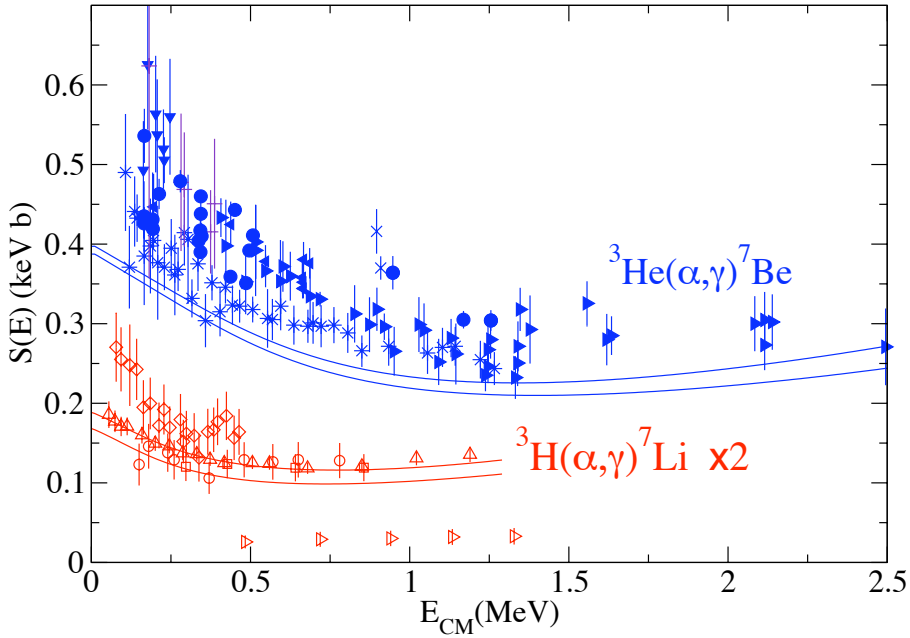
Beyond bound & narrow states: a first pass at nonresonant capture

Several years ago, we computed three (α, γ) cross sections interesting for astrophysics

We:

- avoided off-diagonal GFMC by using VMC bound states
- avoided scattering solutions by using phenomenological correlations $\psi(\mathbf{r}_{12})$ in $\Psi_i \propto \mathcal{A}\Phi_1\Phi_2\psi(\mathbf{r}_{12})$
- concentrated on currents and asymptotic clusterization of final states





Next steps: off-diagonal GFMC matrix elements & scattering states from NN potentials

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 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 some drawbacks to the nodal condition:

- energies have to be evaluated at different box volumes
- for low energies, box has to be enormous

A more flexible approach is an R-matrix boundary condition:

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

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

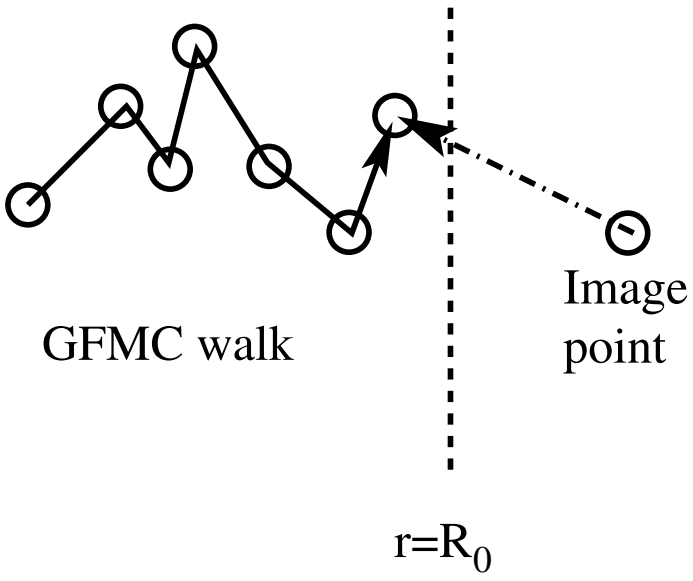
We choose several γ to get states of different $E(\gamma)$, matching asymptotics to find $\delta(E)$

Generalizable to multiple open channels or higher energy with excited-state methods

Implementation of boundary conditions

We can insert either type of boundary condition explicitly into the VMC wave function – build into "single-particle" correlations

Just need to make sure that no pair correlations have long enough range to mess up γ (nodal condition is easy)



In GFMC, we use a method of images

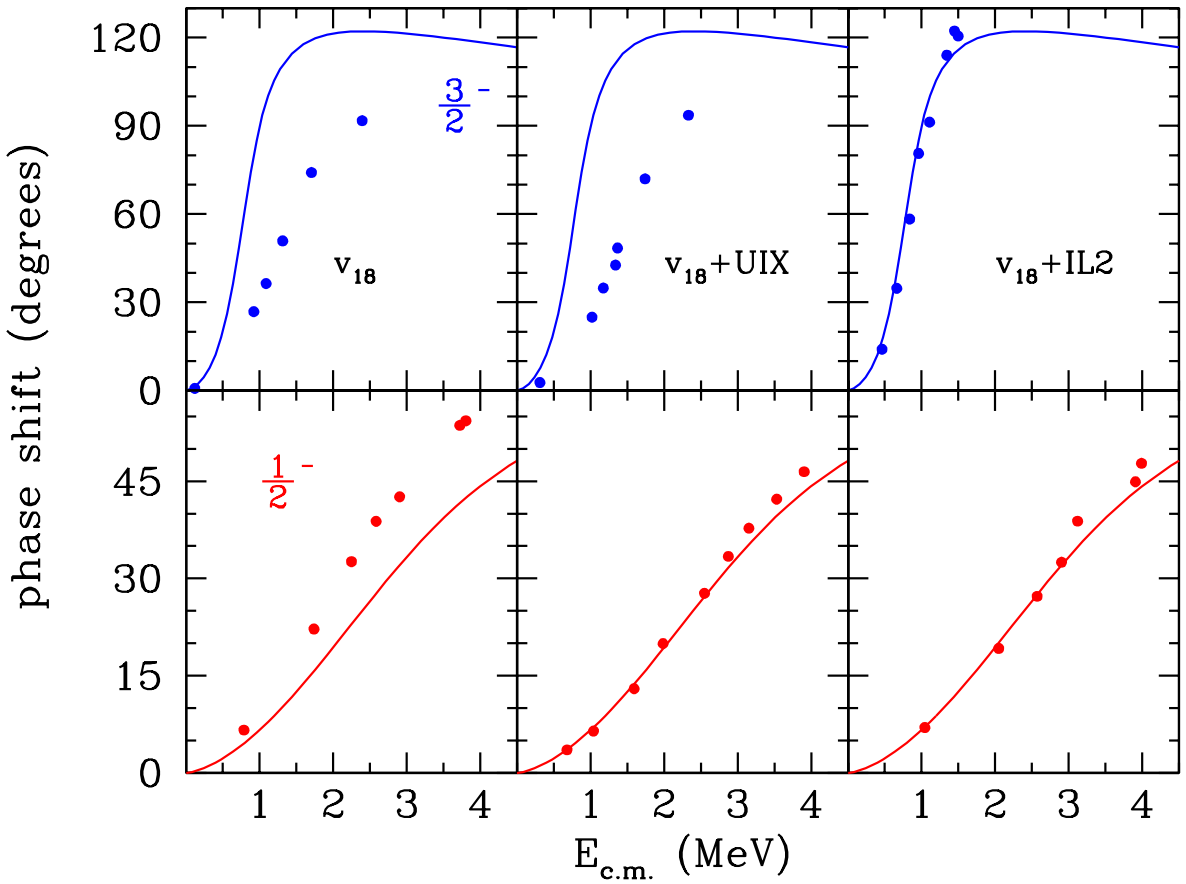
Integral over all space is mapped onto integral inside box using image points with computable locations

Contributions from image points are multiplied by $[1 + \gamma \hat{\mathbf{n}} \cdot (\mathbf{R}_I - \mathbf{R})]$ (or other extrapolation)

Their contributions are added to the propagation of points near the boundary ($\lesssim 0.01$ fm)

First application: ^{5}He

Results illuminate origins of spin-orbit splitting between $3/2^-$ and $1/2^-$ resonances



These are also the first-ever calculations of resonance widths in GFMC

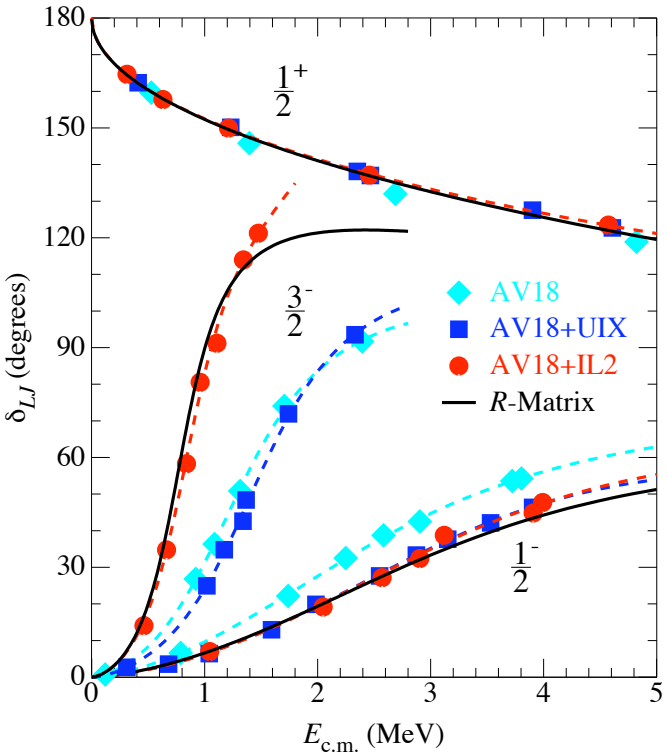
Extraction of S-matrix poles shows agreement with pseudo-bound for $\frac{3}{2}^-$, a few hundred keV difference for $\frac{1}{2}^-$

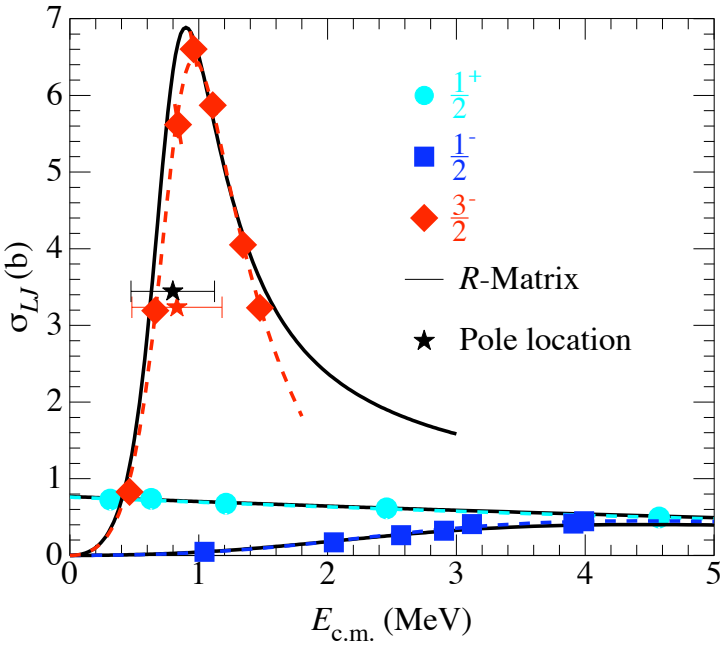
Poles and scattering lengths

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)

Work in progress on $3 + 1$ scattering

^{5}He was expected to be "easy" because there's only one open channel and ^{4}He is compact

^{4}H and ^{4}Li should be only slightly more difficult (easier?)

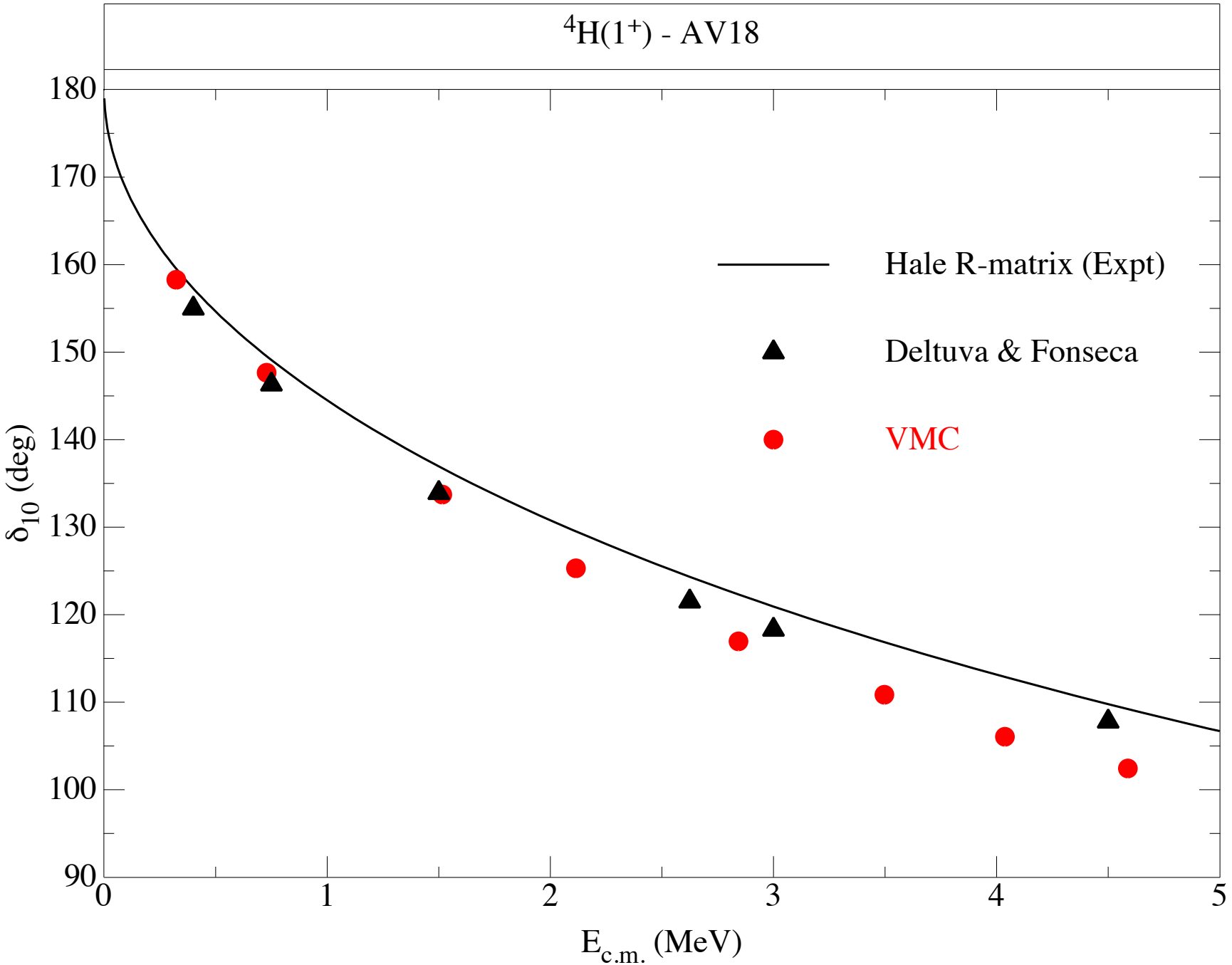
Scattering is $^3\mathrm{H} + n$ and $^3\mathrm{He} + p$

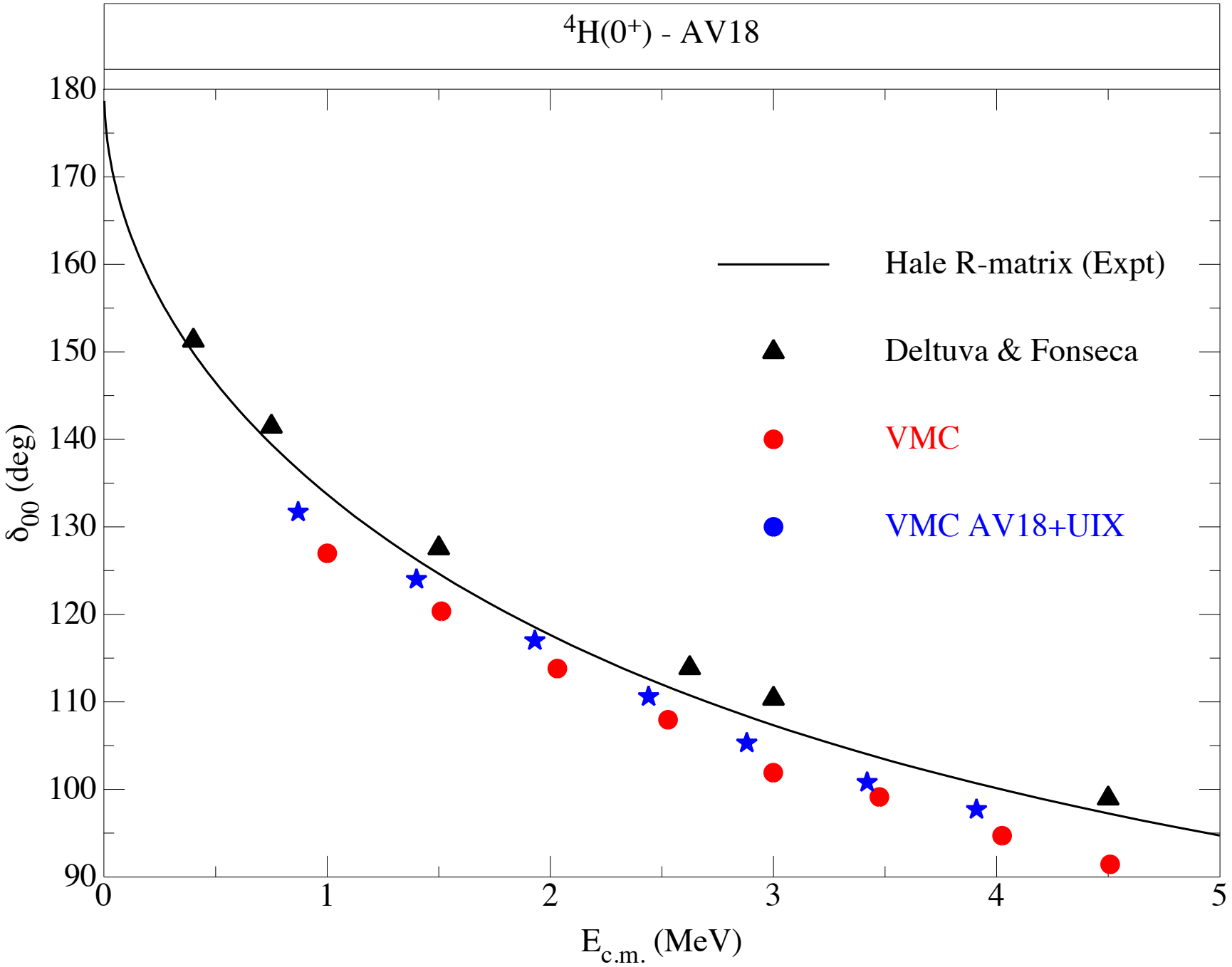
Good for benchmarking against other methods – cf. Arnoldas' talk yesterday & work by the Pisa group

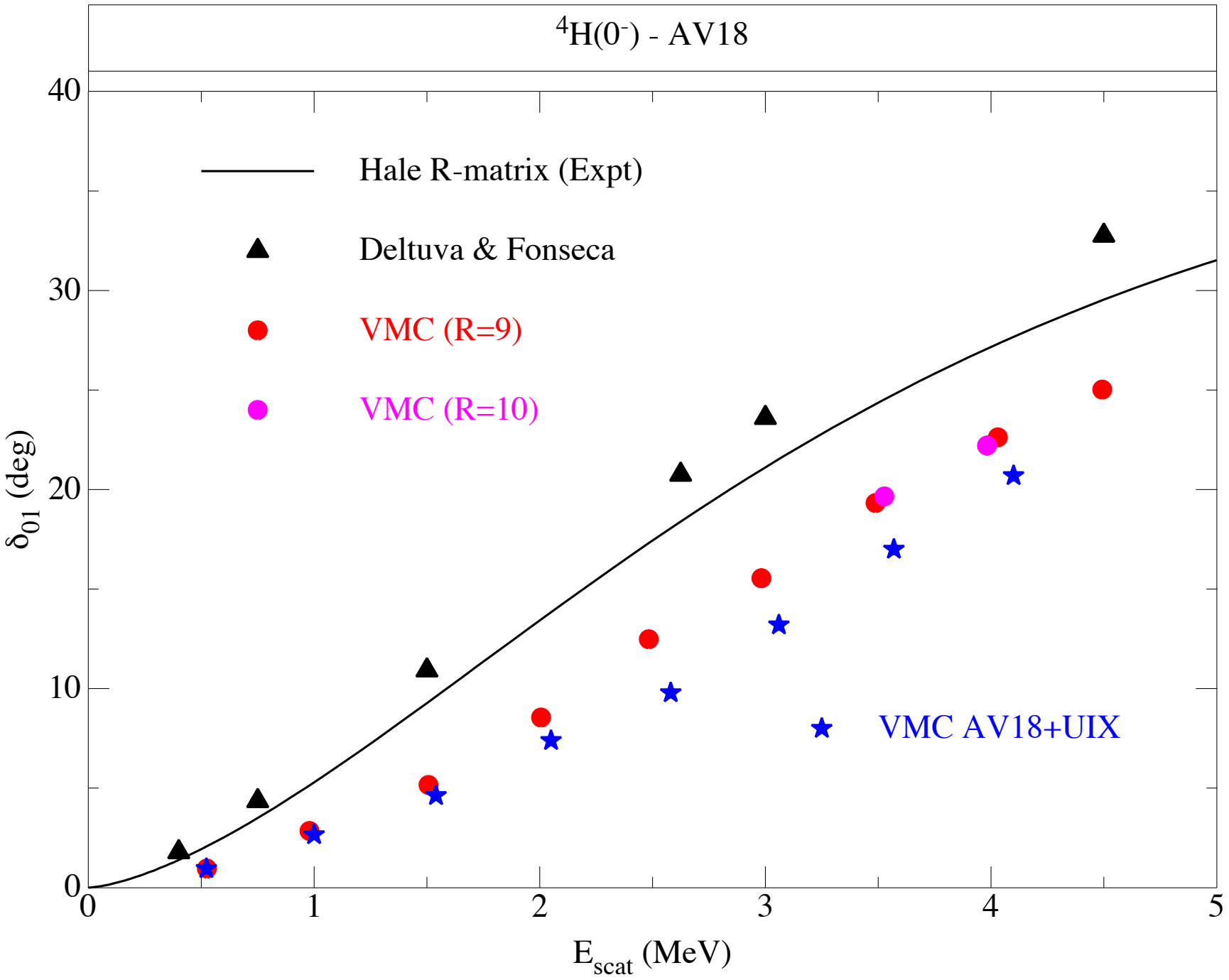
Breakup threshold is relatively high, no underlying bound states

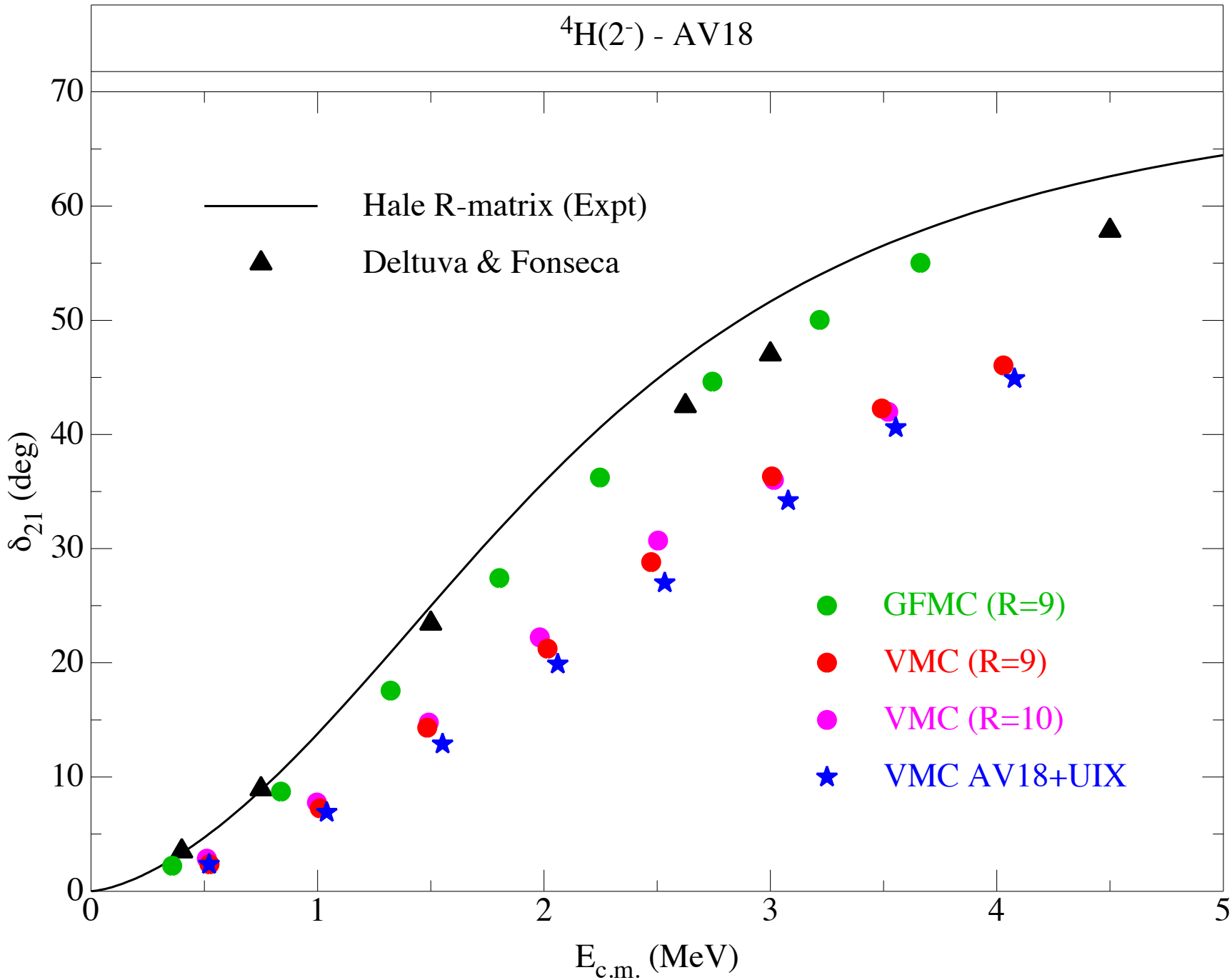
Channel mixing is modest except in 1^- channel

A quick tour of the results so far, all VMC and AV18 alone unless otherwise noted...


^{4}H(1$^+$) - AV18
180
170
160
150
140
130
120
110
100
90
0
1
2
3
4
5
δ_{10} (deg)
$E_{c.m.}$ (MeV)
Hale R-matrix (Expt)
Deltuva & Fonseca
VMC

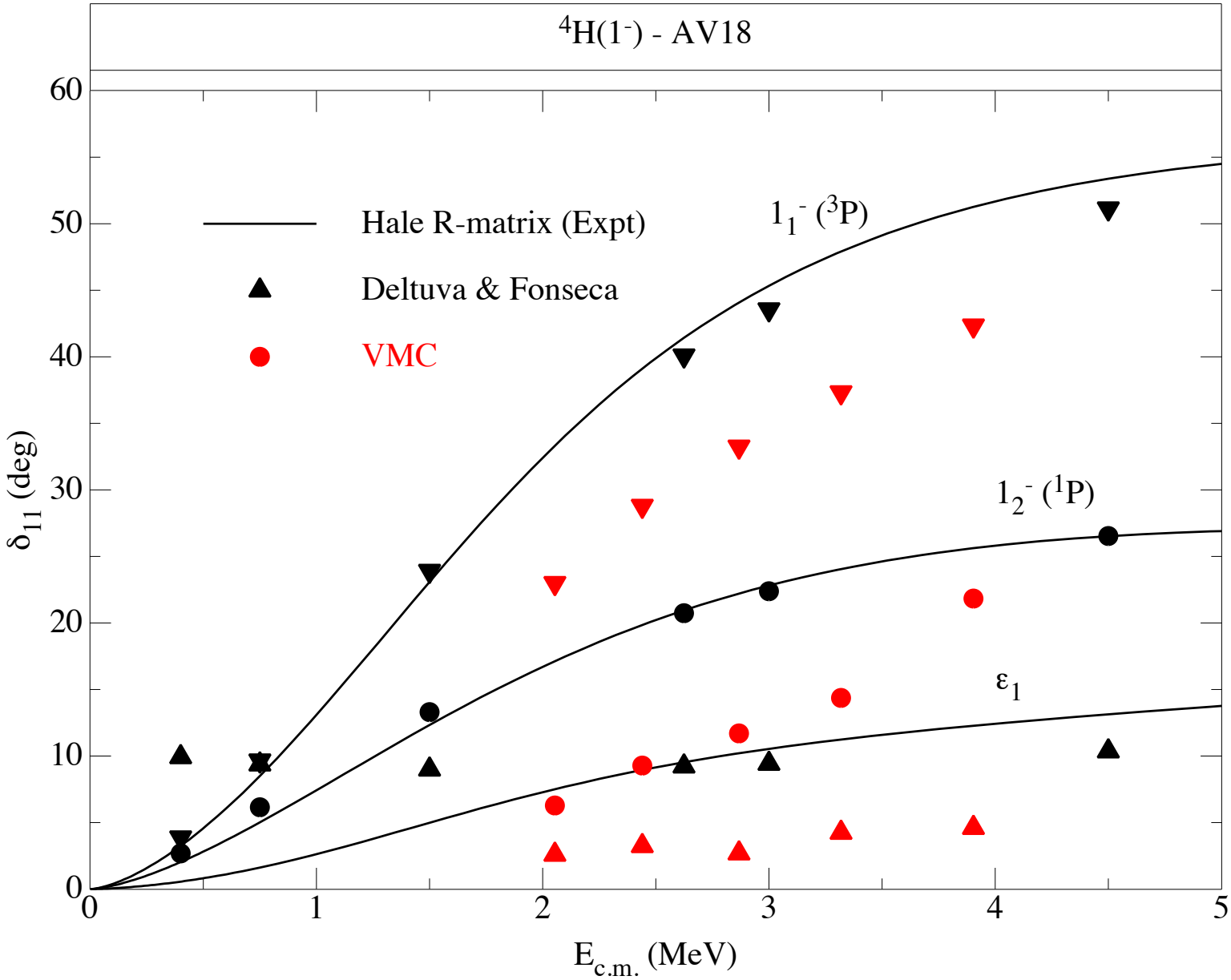

^{4}H(0$^+$) - AV18
180
170
160
150
140
130
120
110
100
90
0
1
2
3
4
5
δ_{00} (deg)
$E_{c.m.}$ (MeV)
Hale R-matrix (Expt)
Deltuva & Fonseca
VMC
VMC AV18+UIX

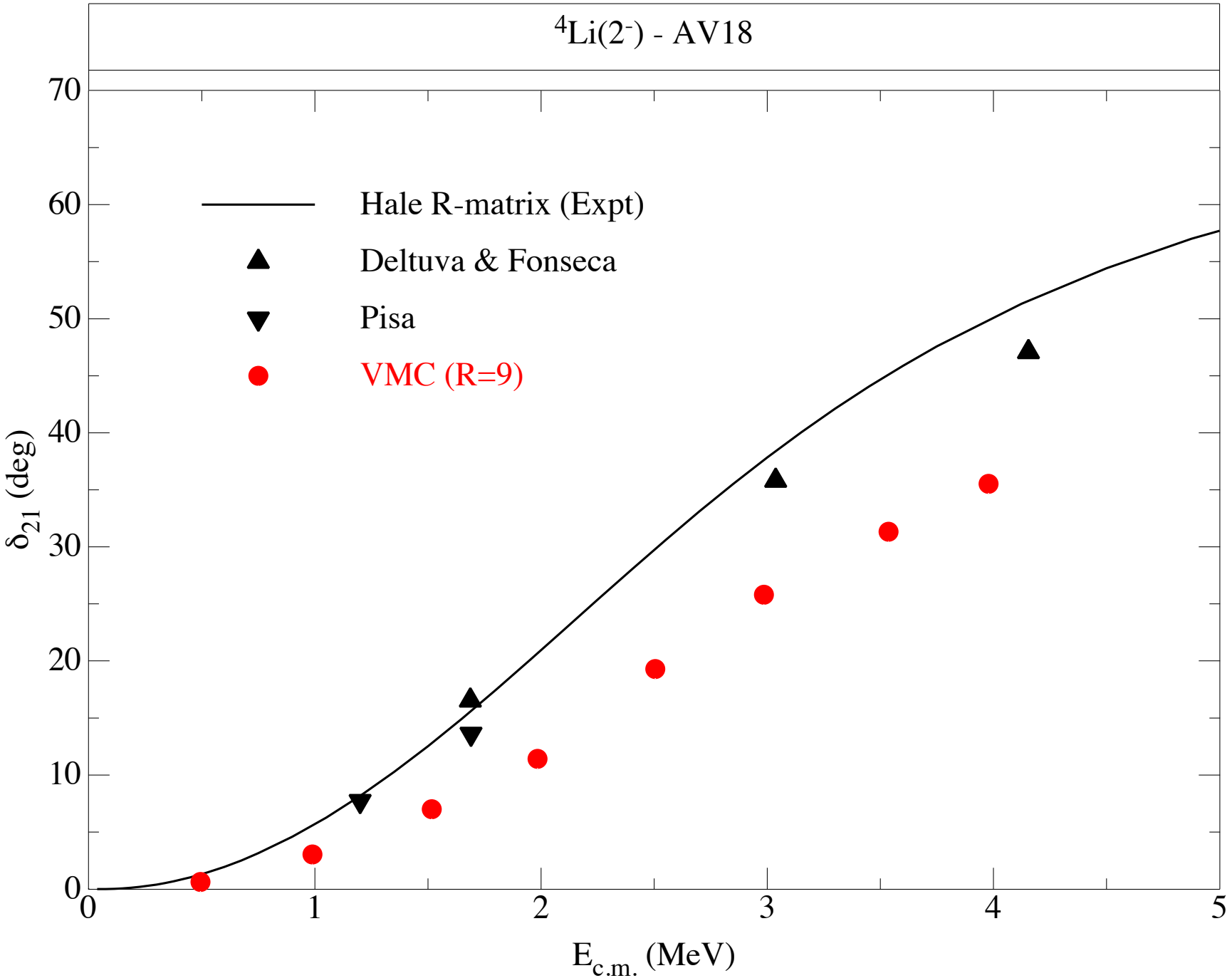

^{4}H(0$^-$) - AV18
Hale R-matrix (Expt)
Deltuva & Fonseca
VMC (R=9)
VMC (R=10)
VMC AV18+UIX
δ_{01} (deg)
E_{scat} (MeV)
0
10
20
30
40
0
1
2
3
4
5



This one was easy to set up for GFMC

For 1^- scattering, singlet & triplet channels mix




^{4}Li(2$^-$) - AV18
Hale R-matrix (Expt)
Deltuva & Fonseca
Pisa
VMC (R=9)
δ_{21} (deg)
$E_{c.m.}$ (MeV)
0
10
20
30
40
50
60
70
0
1
2
3
4
5

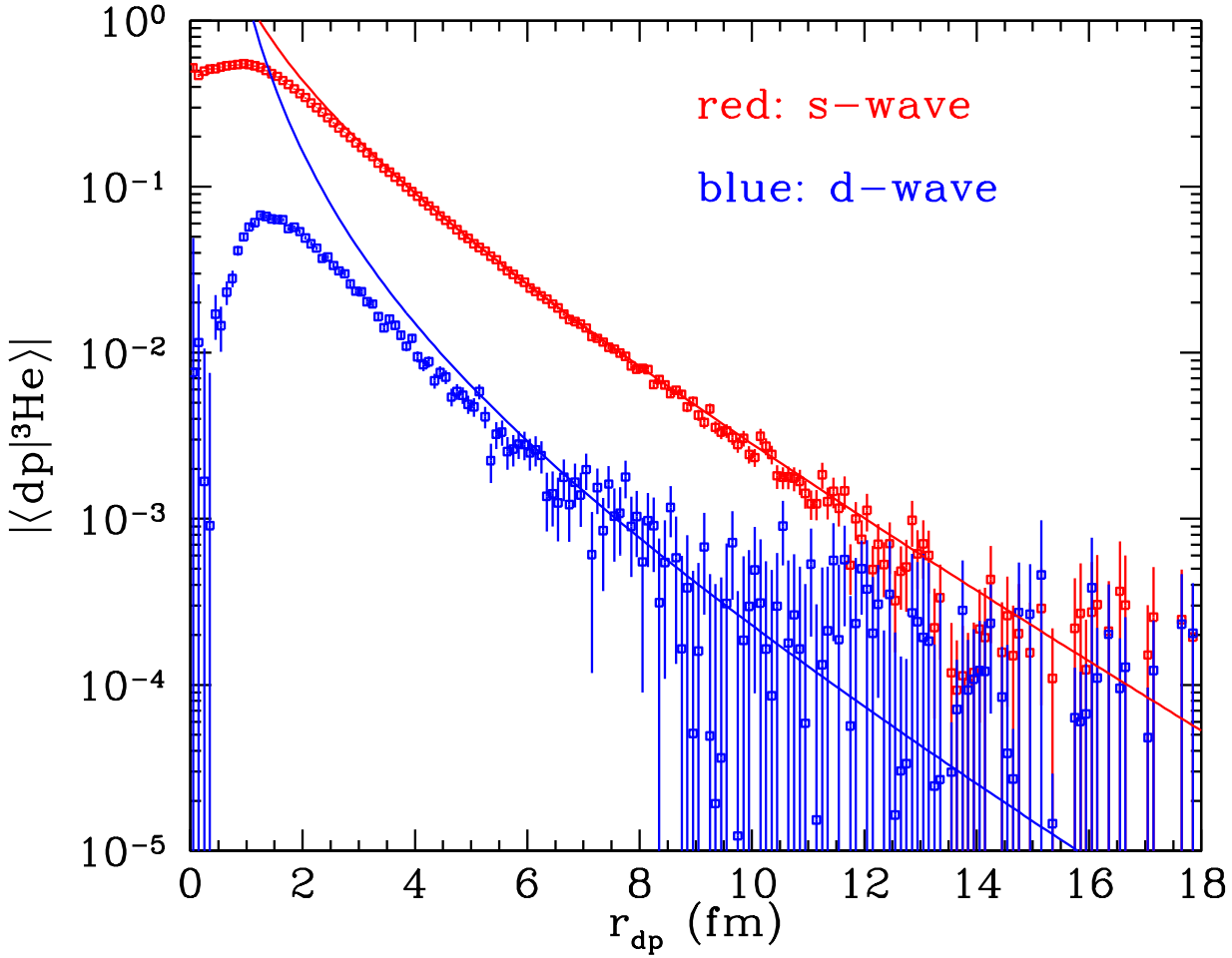
Next steps for scattering

The near-term agenda for QMC scattering is roughly:

- complete $p\,^3\mathrm{He}$ & $n\,^3\mathrm{H}$ scattering calculations with GFMC
- deal with any Coulomb surprises in ^{5}Li, compute ^{5}He parity violation
- resonant (and not) $\alpha\alpha$ scattering and ^{8}Be states
- continued learning on coupled channels, e.g. $n + {}^3\mathrm{He}$, $p + {}^3\mathrm{H}$, $d + d$
- electroweak captures with GFMC
- unbound states previously treated as bound ("successfully" and not)
- continuum lessons applicable to diffuse weakly-bound states?

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 a lot of what happens at the nuclear surface

Surface can get lots of weight in pickup/stripping, so some ANCs are experimentally accessible & sometimes better than spectroscopic factors

Low-energy direct capture can be dominated by these long-range tails

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 can be tricky, especially for small components

Correct asymptotics can be difficult to build into Ψ_T without wrecking good parts of the wave functions – trouble for many observables, including ANCs

There is a smarter way to compute ANCs

Poking around in the tails of the VMC wave functions is not such a smart thing to do

VMC is suited to integrals over wave function interiors

We can take advantage of the Wronskian relation

$$\frac{dM_{-\eta,l+1/2}}{dz}W_{-\eta,l+1/2} - M_{-\eta,l+1/2}\frac{dW_{-\eta,l+1/2}}{dz} = \zeta(\eta,l)$$

to write

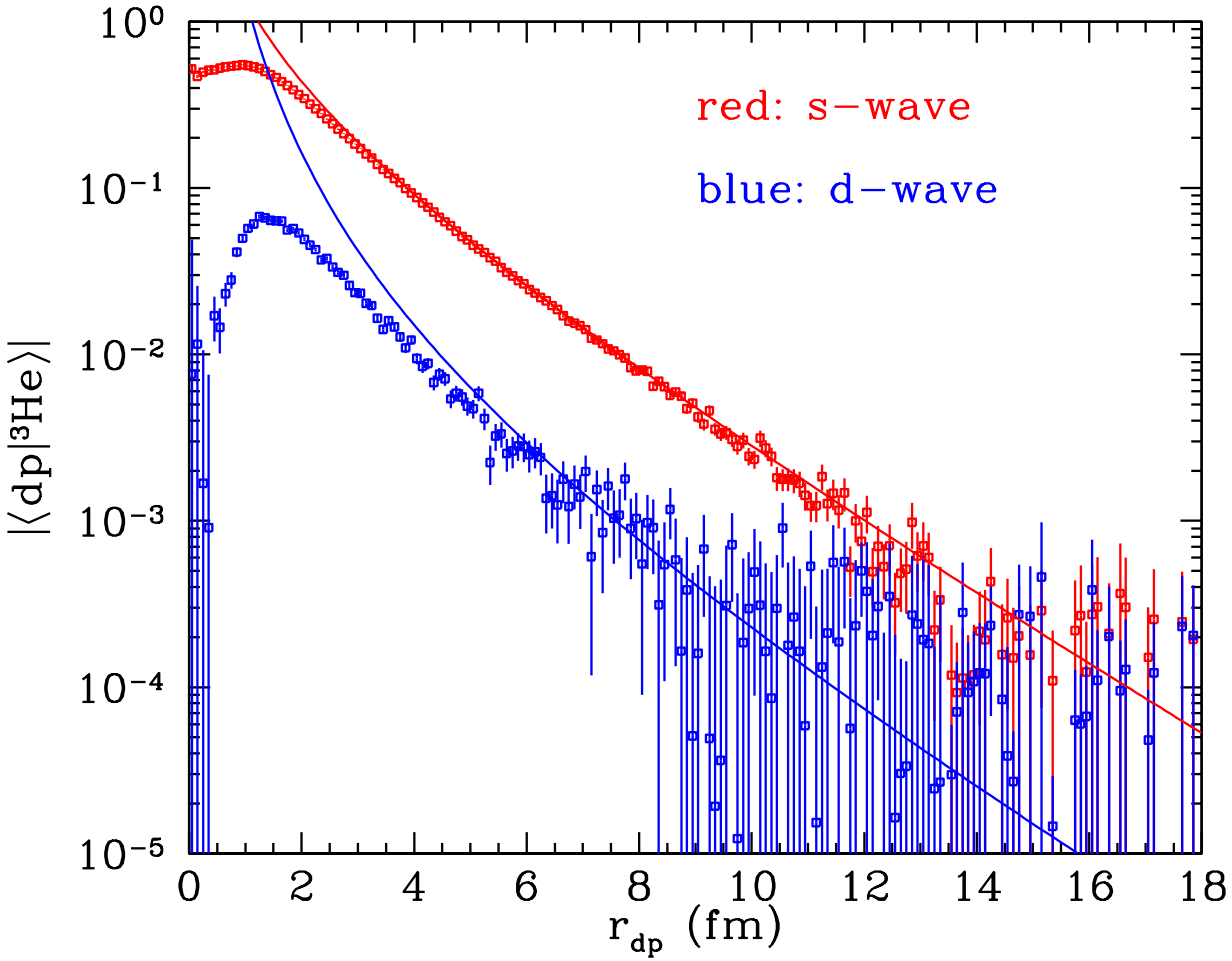
$$C_{lJ}^{12} = \frac{2\mu}{k\hbar^2\zeta}\int M_{-\eta,l+1/2}(2kr)\Phi_1^\dagger\left[\Phi_2^\dagger Y_{lm}(\hat{\mathbf{r}}_{12})\right]_J\left[V_{12} - V_c(\mathbf{r}_{12})\right]\Psi_T d^{3A}r$$

V_{12} contains only terms with nucleons in different clusters, V_c is point-Coulomb interaction between clusters

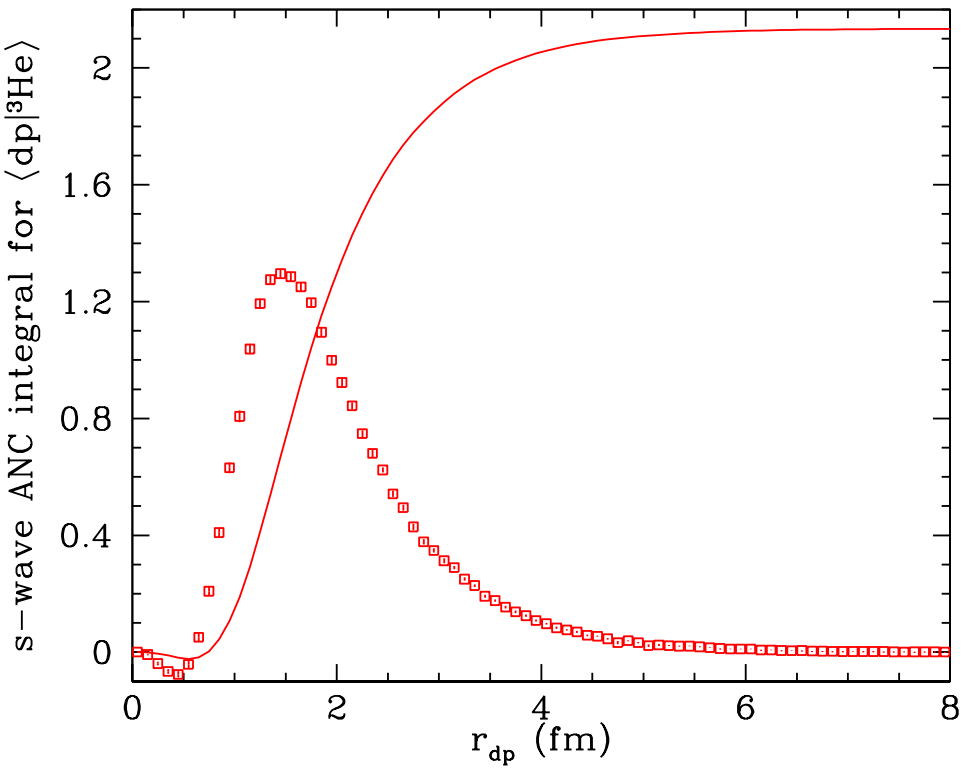
Gell-Mann-Goldberger relation

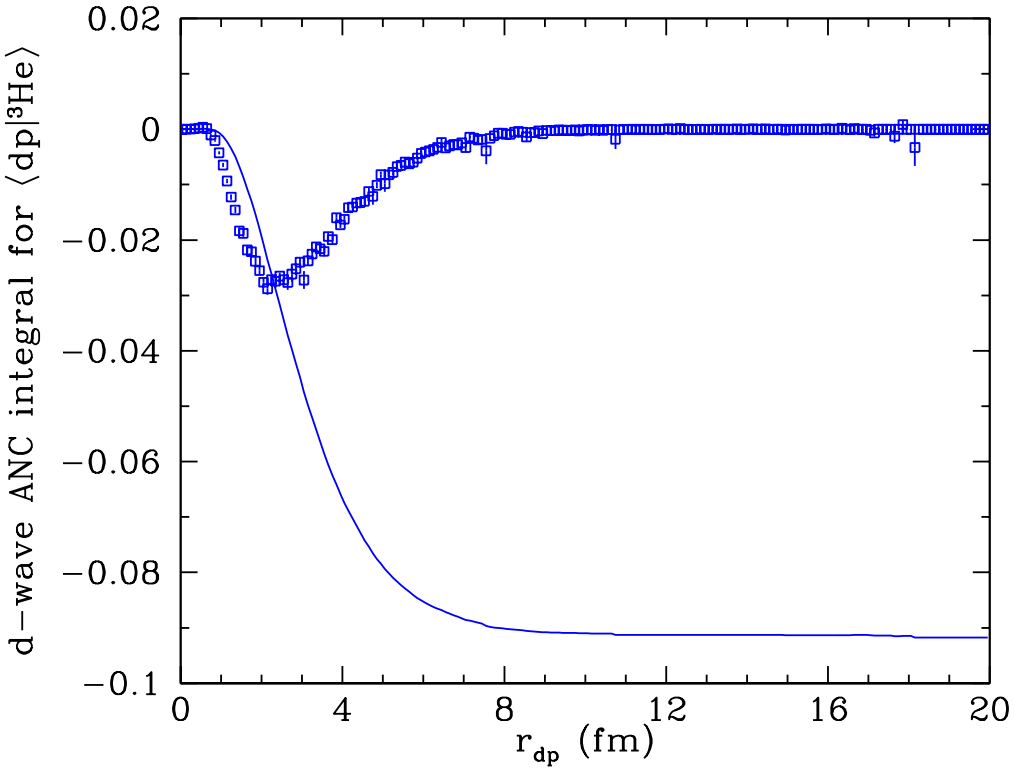
The integral method solves the sampling problem and it should give us better ANCs than we can build explicitly into the Ψ_T

An easy case: ^{3}He $\rightarrow d + p$ with AV18+UIX



is replaced by...





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$^{-1/2}$

This gives $\frac{C_d^{dp}}{C_s^{dp}} = -0.0415(4)$, vs. -0.0389(42) from data compilation

C_d^{dp} converges just where sampling gets sparse in the explicit overlap

Similarly, for ^{3}H $\rightarrow dn$ with AV18+UIX,

$C_s^{dn} = 2.139(8)$ fm$^{-1/2}$, $C_d^{dn} = -0.0971(9)$ fm$^{-1/2}$, for $\frac{C_d^{dn}}{C_s^{dn}} = -0.0454(5)$

The compilation quotes two values,

$$\frac{C_d^{dn}}{C_s^{dn}} = -0.0431(25)$$
$$\frac{C_d^{dn}}{C_s^{dn}} = -0.0411 \pm 0.0013 \pm 0.0012$$

For ^{4}He, we've looked at tails for $n\,^3$He and $p\,^3$H

$$C_s^{pt} = 6.582(23) \text{ fm}^{-1/2}$$
$$C_s^{n\tau} = 6.490(21) \text{ fm}^{-1/2}$$

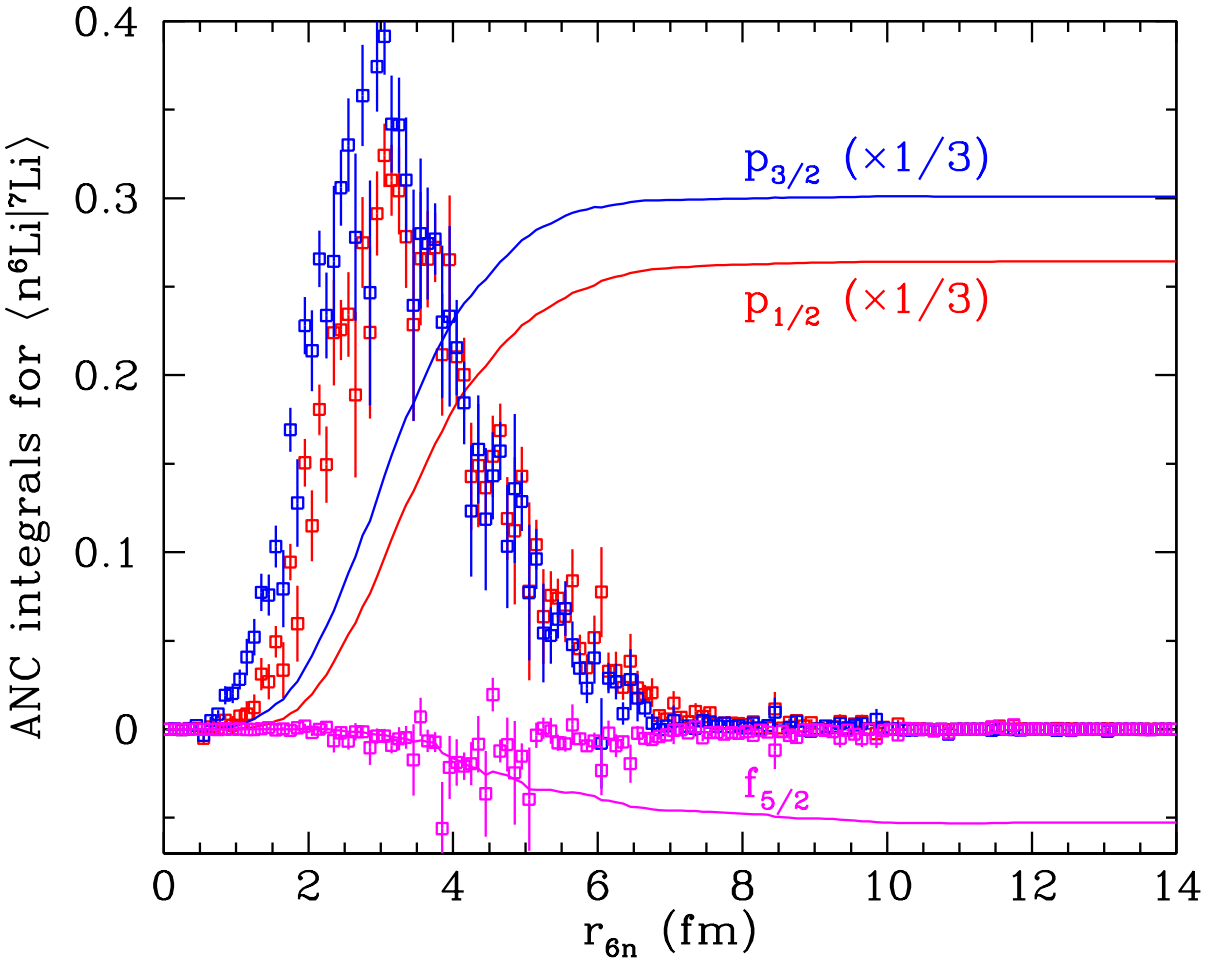
We differ from Pisa by a factor of $\sim \sqrt{8}$ on these, probably a Jacobian

ALL ANCs ARE PRELIMINARY

A harder case (next up in stable $A \to A-1$)

In $A = 3, 4$, the integral approach mainly clears up ambiguity from the overlaps

$^7\mathrm{Li} \to {}^6\mathrm{Li} + n$ demonstrates another kind of case



$$C_{p_{3/2}} = 0.90(2)\ \mathrm{fm}^{-1/2}$$

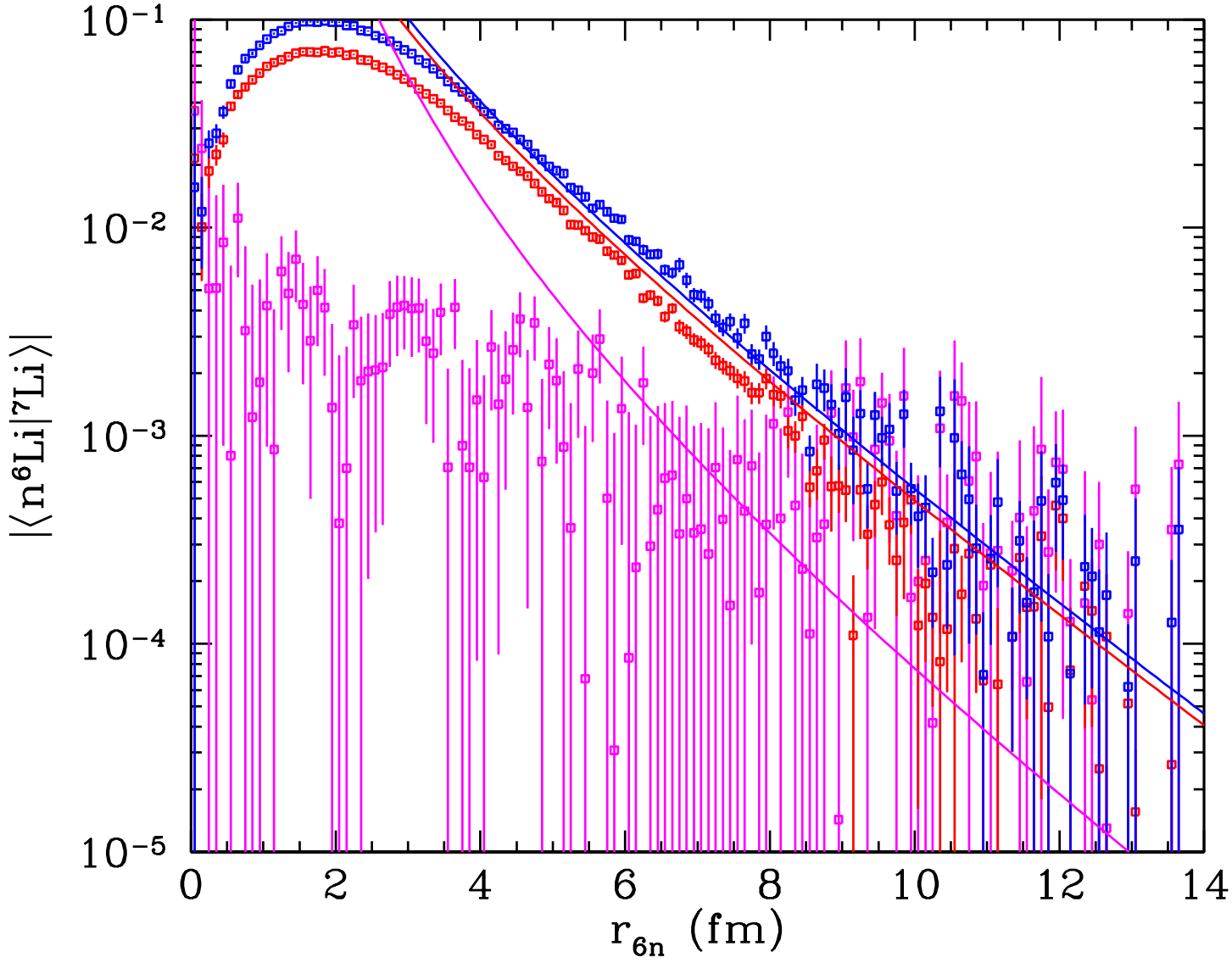
$$C_{p_{1/2}} = 0.79(2)\ \mathrm{fm}^{-1/2}$$

$$C_{f_{5/2}} = -0.053(8)\ \mathrm{fm}^{-1/2}$$

AGAIN, PRELIMINARY

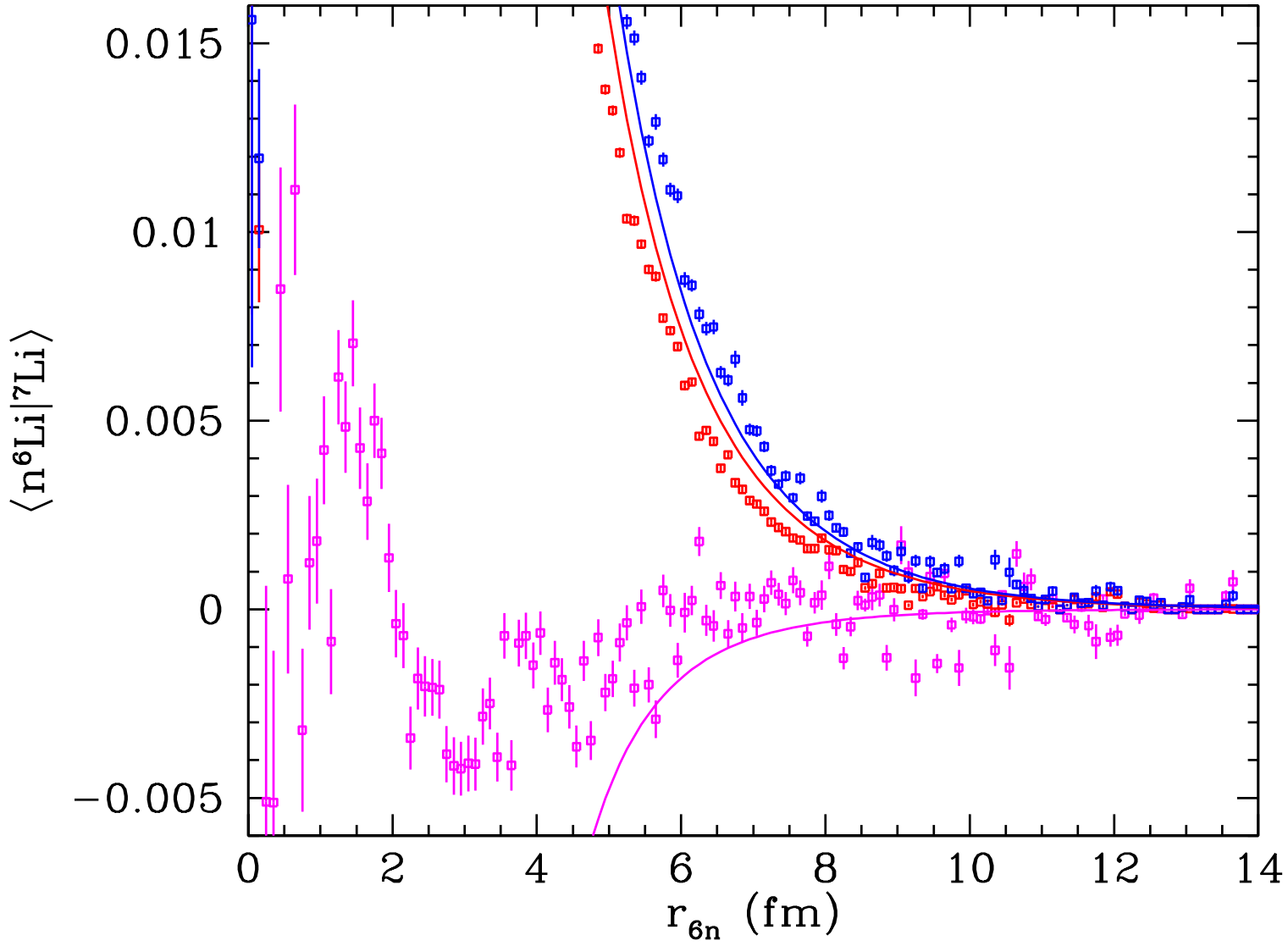
Sadly, these quantities have not been measured

Some things are hard to compute the dumb way



Solid curves are all fixed from an integral ANC calculation with computation time roughly equal to the overlap, none quite what you'd get naïvely

Some things are hard to compute the dumb way



Solid curves are all fixed from an integral ANC calculation with computation time roughly equal to the overlap, none quite what you'd get naïvely

What ANC integrals should be good for

There are several motivations for setting up these calculations now

- a complete set of one-nucleon ANCs for bound states
- cluster-cluster ANCs (e.g. $^7\mathrm{Li} \rightarrow \alpha t$)
- possibility to extract resonance widths from pseudo-bound VMC states
- pointing the way to better variational functions
- extension to GFMC
- extraction of surface amplitudes needed for coupled-channels GFMC
- sometimes more sensible to extract ANCs than spectroscopic factors from data?

This just in: $^8\mathrm{B} \rightarrow {}^7\mathrm{Be} + p$ ANCs

$C_{p_{1/2}} = 0.246(9)\ \mathrm{fm}^{-1/2}$ $\quad C_{p_{3/2}} = -0.691(17)\ \mathrm{fm}^{-1/2}$

$C_{f_{5/2}} = (11 \pm 2) \times 10^{-4}\ \mathrm{fm}^{-1/2}$ $\quad C_{f_{7/2}} = -(11 \pm 5) \times 10^{-4}\ \mathrm{fm}^{-1/2}$

vs. experiment (used an assumed ratio, in agreement with ours),

$|C_{p_{1/2}}| \sim 0.227\ \mathrm{fm}^{-1/2}$ $\quad |C_{p_{3/2}}| = \quad 0.643(33)\ \mathrm{fm}^{-1/2}$