Prospects for Quantum Monte Carlo Calculations of hadronic parity nonconservation in light-nucleus reactions

Kenneth Nollett
San Diego State University

Workshop on Hadronic Parity Nonconservation
KITP Santa Barbara
16 March 2018

A quick introduction to quantum Monte Carlo methods

For VMC/GFMC methods, we do not expand the wave function in basis states, so we don't have to reduce the complicated interaction into a tractable basis

These are two methods that operate on random samples of the wave function in the particle-configuration space $\mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A\}$

The lack of a basis lets us build in strong short-range particle-particle correlations that are difficult in a basis (also avoid spurious center-of-mass motion)

The price is that we don't just diagonalize H once and get lots of eigenvalues

Each nuclear state is a rather separate effort with a separate calculation

Actually it's two separate calculations, as successive approximations

Variational Monte Carlo

Variational Monte Carlo (VMC) is based on a sophisticated guess wave function reflecting pairwise interactions of nucleons:

$$|\Psi_T\rangle = \left[\mathcal{S}\prod_{i<j}(1+U_{ij}+\sum_{k\neq i,j}U_{ijk})\right]\left[\prod_{i<j}f_c(r_{ij})\right]|\Phi_A(JMTT_3)\rangle$$

We evaluate $E_T = \dfrac{\langle\Psi_T|H|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}$, and set adjustable parameters by hand to minimize E_T

Ψ_T originated in calculations of cold nuclear matter (strongly correlated Fermi gas)

VMC does very well in the s-shell, where $|\Phi_A(JMTT_3)\rangle$ is just a Slater determinant in spin/isospin ($\uparrow\downarrow$ np)

In the lower p-shell ($5 \leq A < 12$) it misses by more than 1 MeV/particle (out of 30–100 MeV total binding)

Green's function Monte Carlo

The second method is Green's function Monte Carlo (diffusion Monte Carlo in quantum chemistry, also close to LQCD)

By Monte Carlo integration over a Green's function, we guess $\Psi(0)$ & compute

$$\Psi(\tau) = \exp\left[-H\tau\right]\Psi(0)$$

Any $\Psi(0)$ is a superposition of energy eigenstates, with amplitudes α_i and energies E_i:

$$\Psi(0) = \alpha_0\Psi_0 + \sum\alpha_i\Psi_i \ .$$

Then we have

$$\Psi(\tau) = e^{-E_0\tau} \times [\alpha_0\Psi_0 + \sum\alpha_i e^{-(E_i-E_0)\tau}\Psi_i],$$

and we can see that

$$\Psi_0 \propto \lim_{\tau\to\infty} \Psi(\tau)$$

We use VMC to get $\Psi(0)$ that has only Ψ_0 plus high-energy garbage; GFMC makes that into the ground state

Prometheus unbound

Those methods have been employed with great success in bound states up to $A = 12$

They deal well with hard-core potentials (i.e. AV18) but can handle any potential where nonlocal terms are perturbative

They've mainly been used so far with an implicit square-integrability boundary condition

That limits you to either bound states or narrow unbound states

Relatively little has been done with explicit scattering boundary conditions

Some past QMC calculations of phase shifts

Carlson, Pandharipande, Wiringa (1984)

^{4}He resonances in $t + p$ channel, VMC, nodal boundary condition

Carlson, Schmidt, Kalos (1987)

$n\alpha$ p-wave scattering ($\frac{1}{2}^-$, $\frac{3}{2}^-$), VMC, nodal boundary condition

Carlson (1990s)

Early efforts at ^{5}He GFMC?

Nollett, Pieper, Wiringa, Carlson, Hale (2007)

$n\alpha$ scattering $\frac{1}{2}^+$, $\frac{1}{2}^-$, $\frac{3}{2}^-$, GFMC, log derivative boundary condition

Lynn et al. (2016 & 2017)

$n\alpha$ p-wave scattering, GFMC, log derivative(?) boundary condition

Radiative captures, VMC bound states, phenomenological initial states

For these, VMC was used for the bound states

Unbound cluster-cluster correlations came from a phenomenological "optical" potential

Arriaga, Pandharipande, Schiavilla (1991)

$^2\mathrm{H}(d,\gamma)^4\mathrm{He}$

Nollett, Wiringa, Schiavilla (2001a)

$^2\mathrm{H}(\alpha,\gamma)^6\mathrm{Li}$

Nollett (2001)

$^3\mathrm{H}(\alpha,\gamma)^7\mathrm{Li}$ and $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$

Probably fair to call these cases of mixed success

Quantum Monte Carlo: the nodal boundary condition

Quantum Monte Carlo methods are (more or less) variational: they produce the lowest energy level satisfying the imposed constraints

Application to scattering so far sets up an eigenvalue problem with the ground state as the desired state

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

Find energy of

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

evaluated only at $r_{12} < R_0$

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

Improving on the nodal boundary condition

But then different energies are evaluated at different box volumes: lose some ability to compute differences (e.g. stored walks)

At low energies, the box must be enormous, & calculation is mostly noninteracting clusters

An R-matrix boundary condition avoids these drawbacks

For single-channel scattering, specify a channel radius R_0 & a logarithmic derivative γ:

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

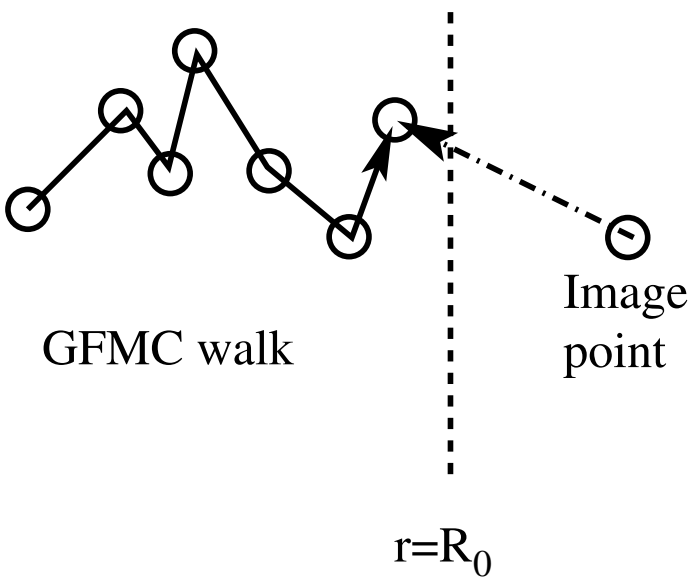
Then fix R_0 at some "small" value (beyond nuclear radius and nucleon exchanges)

Vary the chosen γ to get states of different E, match asymptotics to find $\delta(E)$

Implementation of boundary conditions

Either type of boundary condition can be built into the VMC wave function – we used the "single-particle" correlations in ^{5}He

Just need to make sure that none of the pair correlations have long enough range to mess up γ (nodal condition is easy)



In GFMC, we use Joe's 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

We assumed configurations with one particle $\gtrsim R_0$ from c.m. of other 4 are entirely in the αn channel (must clip the α a bit)

First time out with GFMC: parity-conserving n ^{4}He

We chose ^{5}He as the first system to try this out

^{4}He is compact and symmetric ($J = 0^+$), no excitations or thresholds for 20 MeV above ground state

We still learned a lot

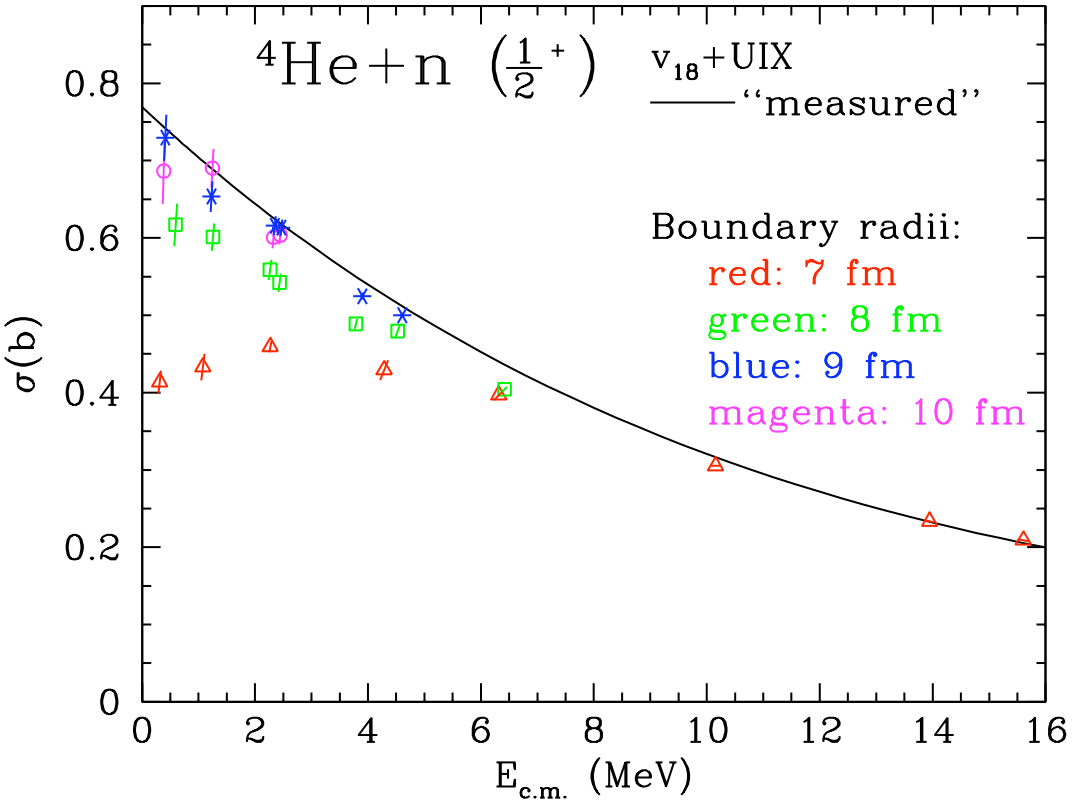
Low-energy scattering is tougher than energy levels because we need small energy differences from a threshold, not absolute energy

A lot of details needed attention to make it work & give $\delta(E)$ that I believed

Large radius was needed to avoid exchange effects

The box radius R must be located beyond any interaction & exchange between ^{4}He & scattering neutron

As R increases, less of the box volume is "interesting" & the maximum energy we can compute gets smaller



$R = 7$ fm is not large enough

$R = 9$ fm is large enough

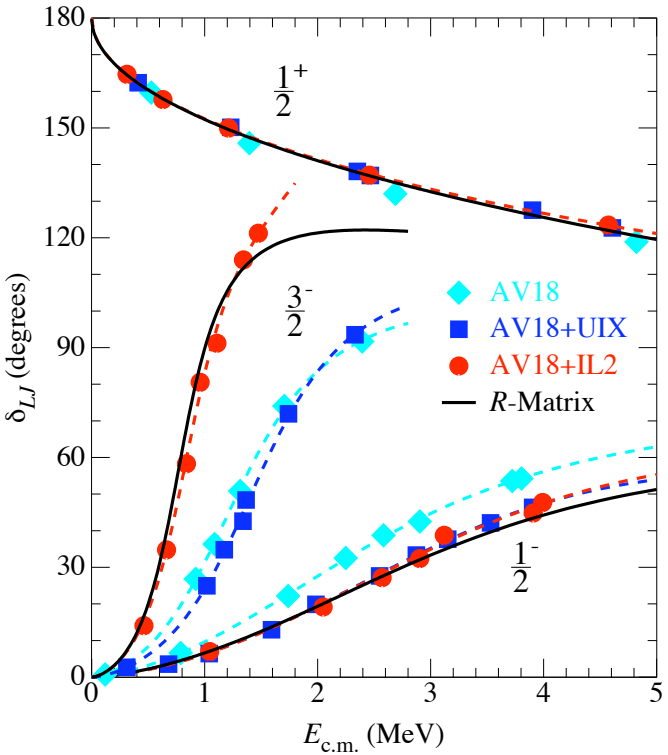
But then highest single-node s-wave state in box is ~ 4.5 MeV

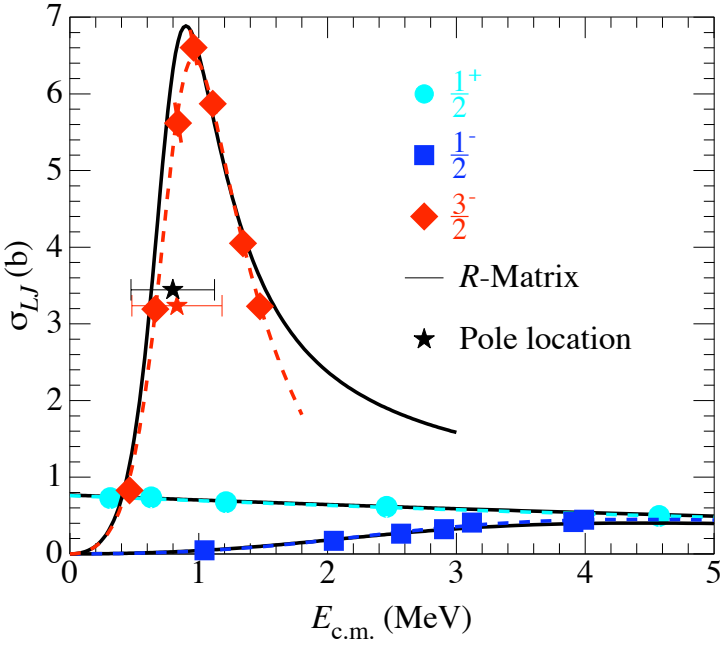
Poles & scattering lengths

s-wave turns 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	$0.798 - 0.324i$	$2.07 - 2.79i$





Phase shifts show the role of NNN potential
in spin-orbit splitting

Steve Pieper also fitted pole locations just
like you would do with experimental data

Some first attempts at $3 + 1$ scattering

^{5}He was expected to be "easy" because there's only one open channel, ^{4}He is compact, scattering channel similar to VMC structure

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

$A = 4$ would also allow a check against HH & AGS calculations

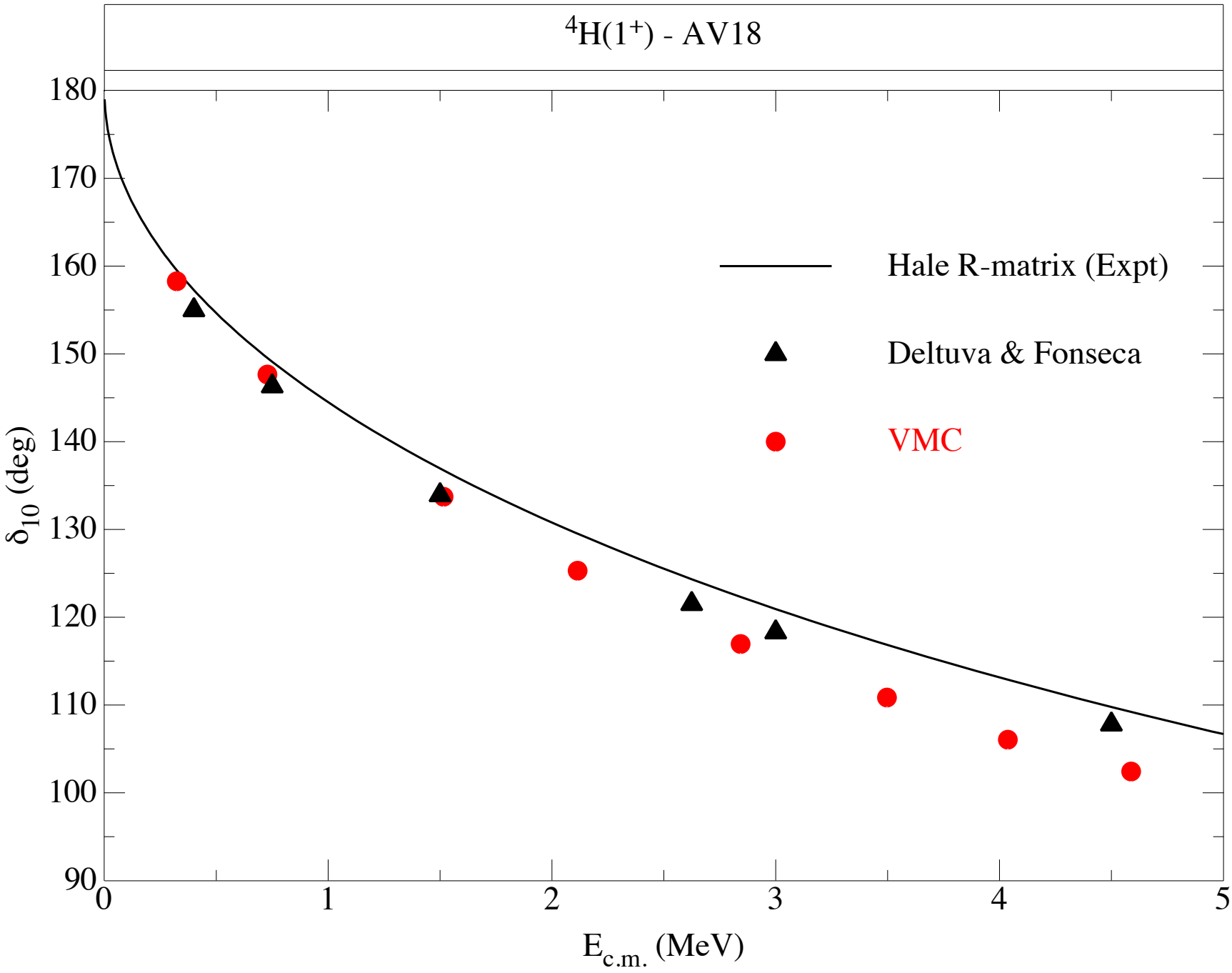
Bob Wiringa & I started on scattering in $^3\mathrm{H} + n$ and $^3\mathrm{He} + p$ a few years ago but got diverted

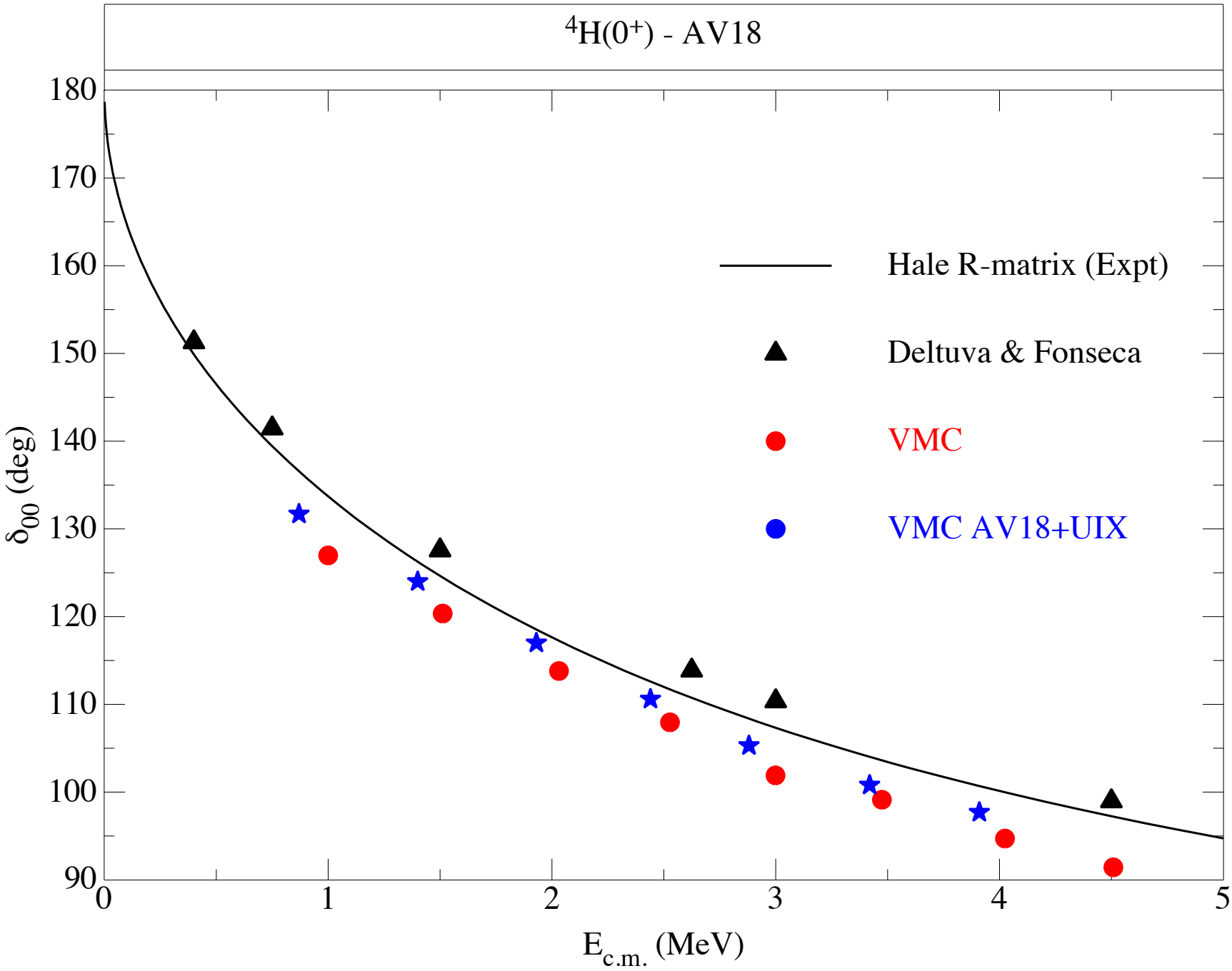
Breakup threshold is relatively high, no underlying bound states

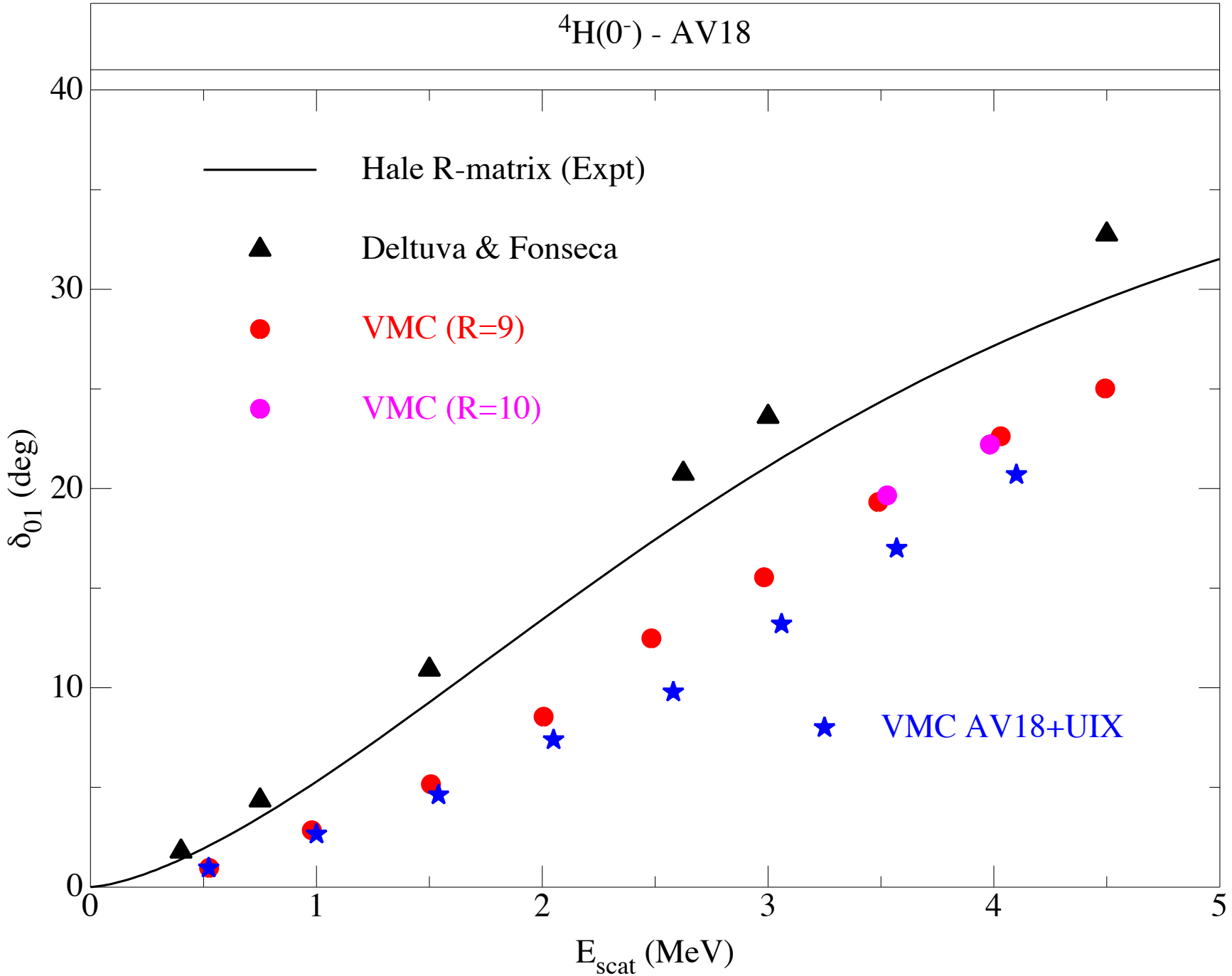
Channel mixing is modest except in 1^- channel

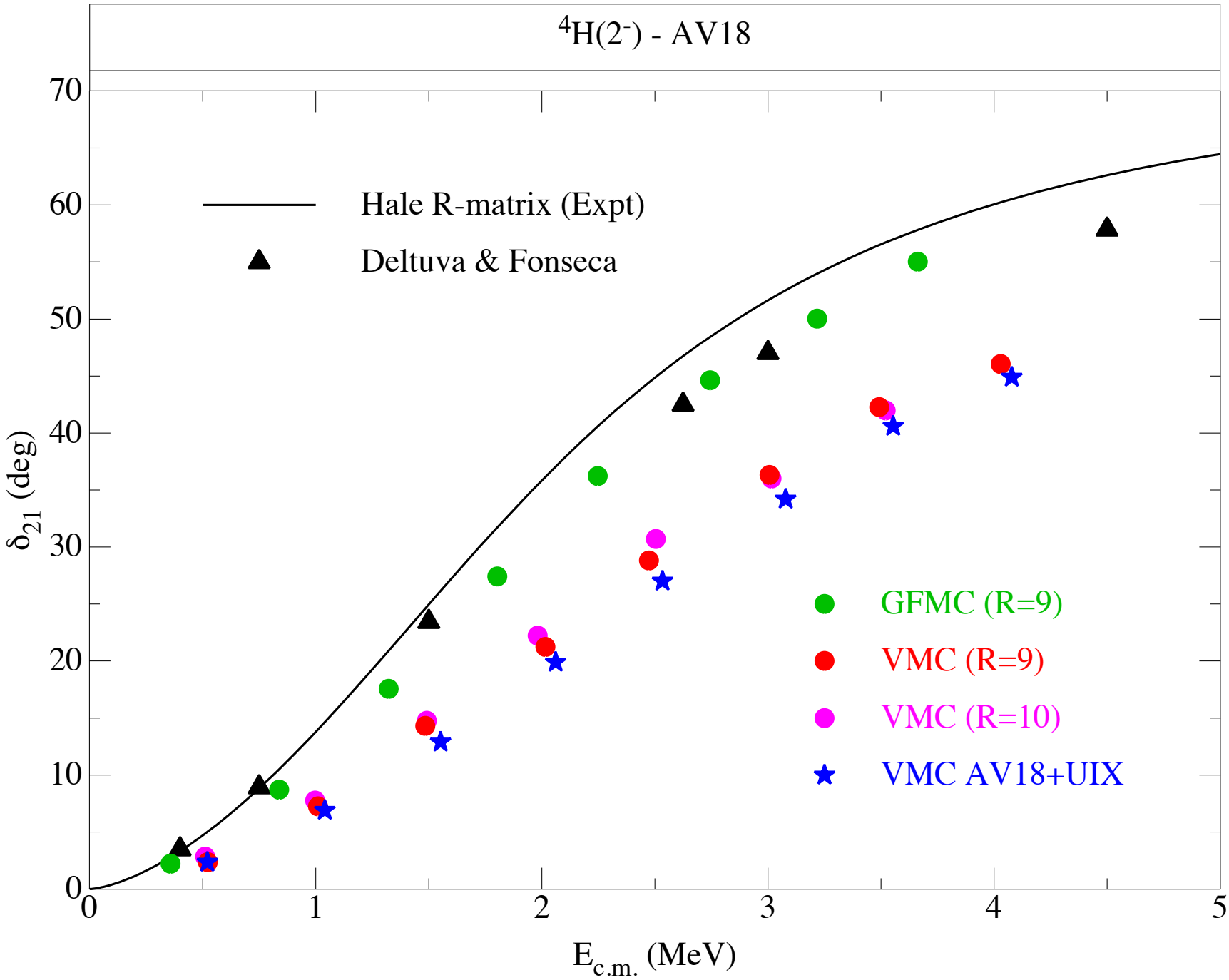
I have a PhD student starting on this now, with the main goal of learning to do coupled channels in $J = 1^-$

A quick tour of what we found, all VMC and AV18 alone unless otherwise noted...

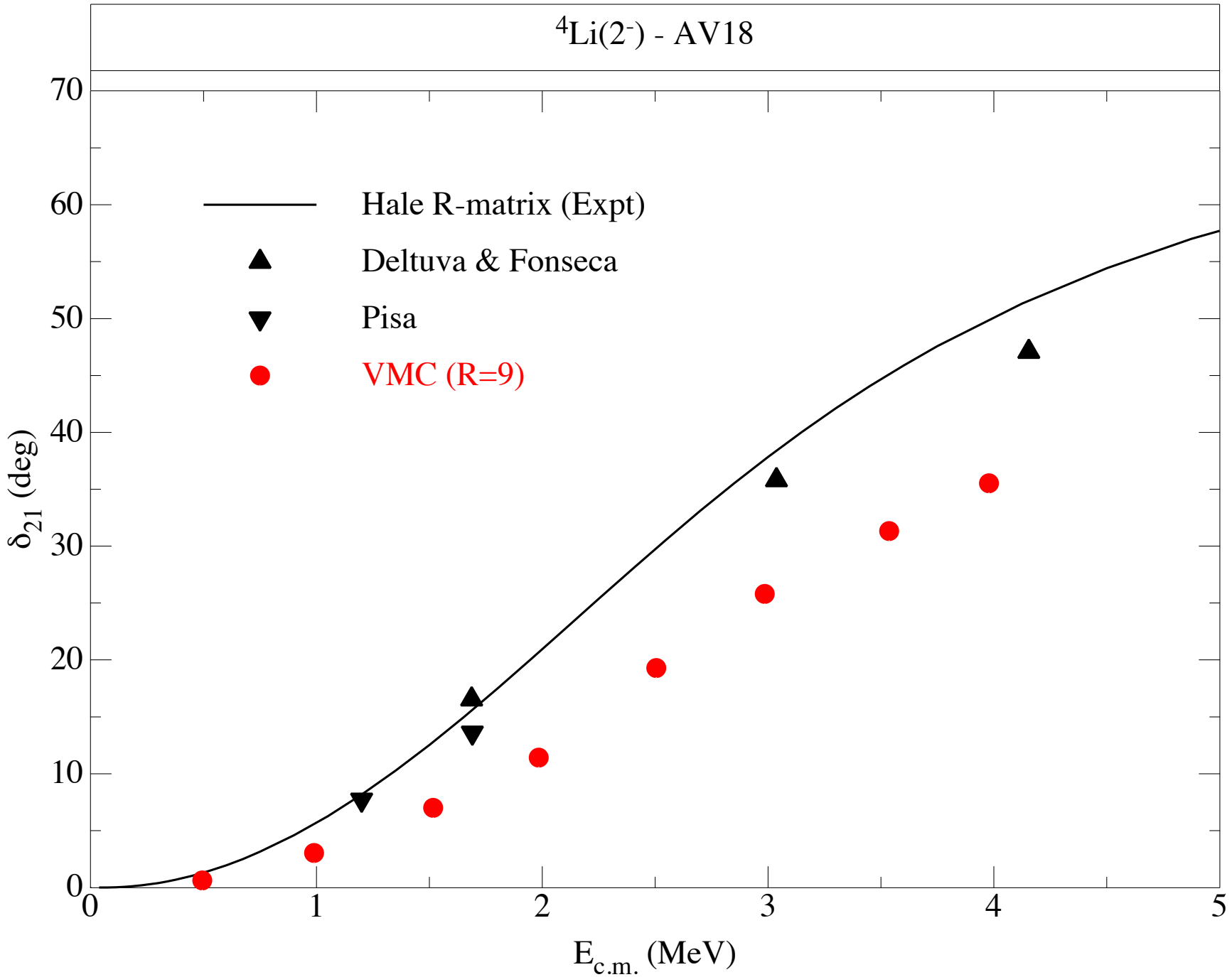

^{4}H(1$^+$) - AV18
180
170
160
150
140
130
120
110
100
90
0
1
2
3
4
5
δ_{10} (deg)
$E_{c.m.}$ (MeV)
Hale R-matrix (Expt)
Deltuva & Fonseca
VMC


^{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


^{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

Spin rotation in $n\,{}^4$He

There was a start on $n + {}^4$He spin rotation in $\sim$ 2010

Ana Arriaga & Rocco Schiavilla did a bunch of work on operators

Probably you could just take the lowest-energy s- & p-wave states from my ^{5}He paper & compute a matrix element

$$\frac{1}{\rho}\frac{d\phi}{dz} = \frac{16\pi}{v_{\rm rel}}\,{\rm Im}\left[{}^{(-)}\left\langle {}^2P_{1/2}, J_z \left| v^{\rm PV} \right| {}^2S_{1/2}, J_z \right\rangle^{(+)}\right]$$

I spent some time trying to get states as close to threshold as I could

The real problem to be solved is to normalize the wave function

$$\left| {}^{2s+1}L_J, J_z \right\rangle^{(\pm)} \longrightarrow \mathcal{A}\phi_\alpha \left[Y_L^M \otimes \chi\right]_{JJ_z} \times e^{\pm i\delta_{JL}} \left[\cos\delta_{JL} F_L(kr) + \sin\delta_{JL} G_L(kr)\right]$$

Normalizing the wave function

Single-channel phase shifts just need wave functions normalized to unity over the box volume

Then phase shifts come from $\langle H \rangle$ & the log-derivative boundary condition

Now we need waves normalized to incoming & outgoing unit-flux waves:

$$\left| {}^{2s+1}L_J, J_z \right\rangle^{(\pm)} \longrightarrow \mathcal{A}\phi_\alpha \left[Y_L^M \otimes \chi \right]_{JJ_z} \times e^{\pm i\delta_{JL}} \left[\cos\delta_{JL} F_L(kr) + \sin\delta_{JL} G_L(kr) \right]$$

This comes down to specifying the wave function amplitude at the box surface

Some possibilities:

1. Read density from Monte Carlo samples in a thin shell (noisy)
2. Compute as Lippmann-Schwinger integral over interior (needs machinery)

2.5 Just build v^{PV} into Lippmann-Schwinger & use ratio somehow?

3. Build into GFMC boundary condition somehow?

Current status

Thin-shell norm depended more than I liked on how I defined shell & averaging

I was working on Lippmann-Schwinger integral for bound-state ANCs at the time & planned to fold that in

There followed a few years when I focused on problems unlikely to hit snags

Now I'm more interested in building up QMC scattering/reaction methods than applying what I already have, especially with limited labor force

Some collaboration rebuilding would also be needed: I need a v^{PV}

I suspect that the eventual calculation will contain a lot of cancellation:

Antisymmetry requires a node in the projection of s-wave states into the αn channel

What about $p\,^4$He?

Close to threshold, this is the same as $n\,^4$He – just an isospin rotation away

I have preliminary phase shifts for P-conserving $p\,^4$He somewhere

The existing PV measurement is at $\bar{E} = 45$ MeV lab (36 MeV c.m.) – WHY??

I can't do that as the ground state in a box

It may need more > 5 box states in a minimal-size box

I'd also be happier below the breakup threshold (20 MeV c.m.)

At ~ 5 MeV, I could do it just as easily as n spin rotation

Would Rutherford make that impossible experimentally?
Provide useful interference/amplification?

Thinking outside the box

I could also abandon exact solution & use accurate ^{4}He in more exact version of old calculations

Roser & Simonius $p\,^4\mathrm{He}$ can be viewed as DWBA with a very crude version of the VMC ^{4}He (looks to me like it has exchange, BTW)

So that's something I could do more or less immediately with variational ^{4}He (given time & maybe a sharp student)

It would look a lot like the radiative captures I did as a student

Same comment maybe applies to n spin rotation

But should I want to do that? Enough of an improvement to be worthwhile? Bad for my brand?