

# Some Quantum Monte Carlo calculations of continuum properties in light nuclei

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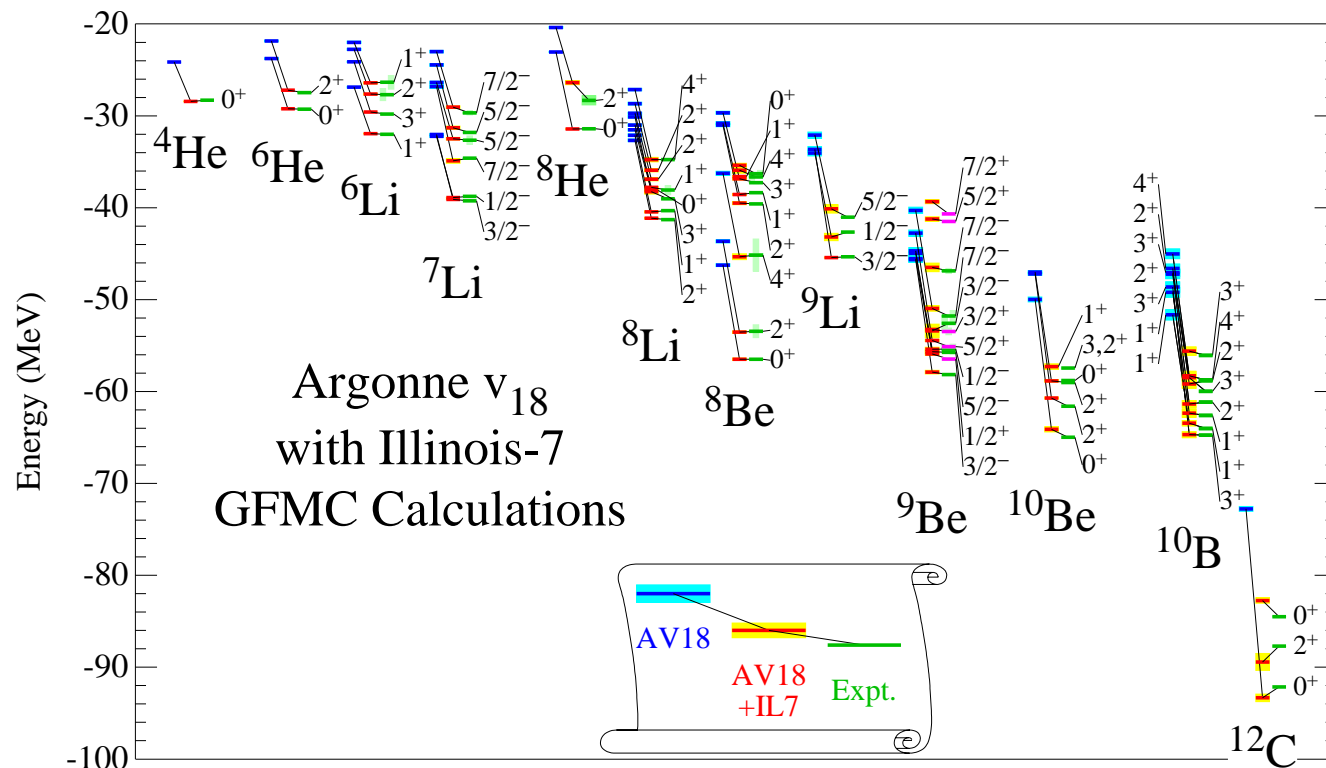
Advances in Monte Carlo Techniques for Many-Body Quantum Systems

Institute for Nuclear Theory

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## Ab initio nuclear physics in the continuum

Nuclear calculations from quantitatively realistic Hamiltonians have focused on bound-state properties



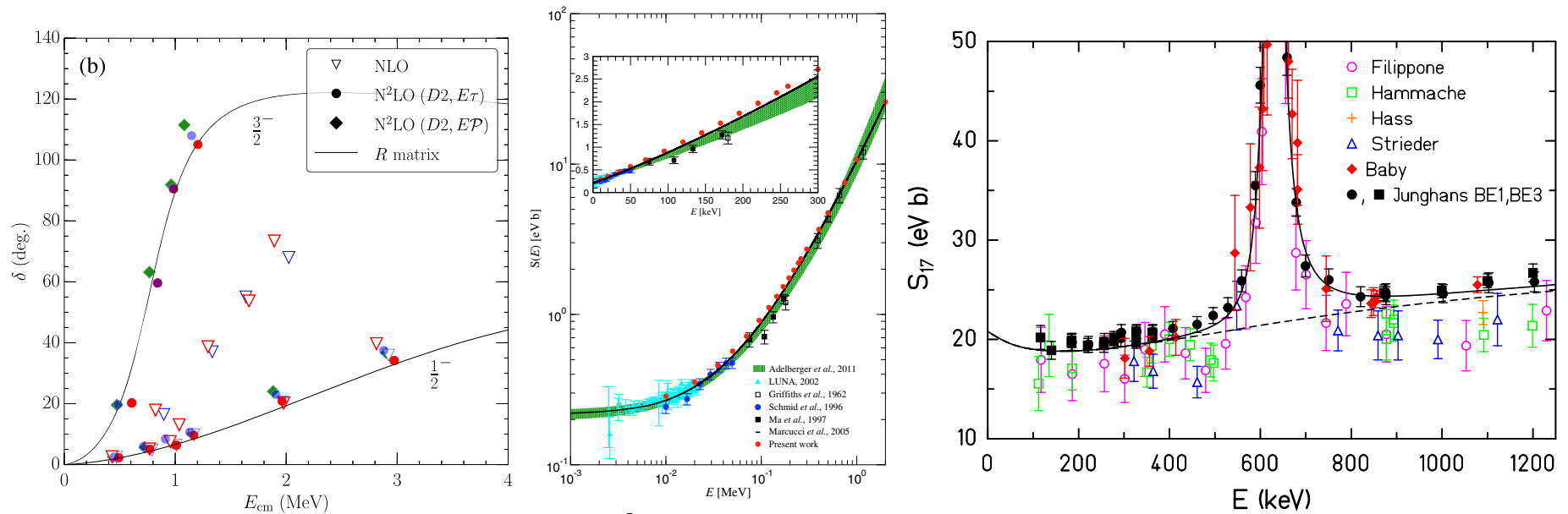
Carlson et al. (2015)

Even the resonances here have been treated as bound states here for computation

# Ab initio nuclear physics in the continuum

But there is also useful information in nuclear collisions

They probe the nuclear Hamiltonian, and cross sections are needed for astrophysics & other applications



${}^5\text{He}$  phase shifts: Lynn et al. (2016)

$d(p, \gamma){}^3\text{He}$ :  
Marcucci et al. (2016)

${}^7\text{Be}(p, \gamma){}^8\text{B}$ : Adelberger et al. (2011)

There is a lot of recognition (e.g., the 2015 Long-Range Plan) that *ab initio* reaction theory is an important direction for the near future

But relatively little has happened so far (exceptions: Quaglioni et al., Lee et al.)

## Why has so little been done?

Bound state boundary conditions are easy: just use  $L^2$  (really,  $L^p$ ) basis/variational functions

Your basis functions or variational ansatz may be poor in the wave function tails

But then the tails are typically small, unimportant for many observables, irrelevant for energy-driven methods

You just do your CI diagonalization / variational minimization / GFMC projection on  $L^p$  functions and get good binding energies

Sufficiently narrow resonance wave functions are “nearly”  $L^p$ , so at least energies are computable with bound-state techniques

## Why has so little been done?

Scattering is different because you only care about the tails

You could (always using stationary states):

Impose a boundary condition in each channel & diagonalize  $H$

Use the Bloch operator ( $\sim$  Lagrange multiplier enforcing a log derivative)

Solve Kohn or Schwinger variational principle to find  $K$ -matrix

Set up RGM equations or adiabatic potential & compute channel wave functions

Formulate the problem as the Lippmann-Schwinger equation, maybe using some form of Born approximation

I'm mainly working on the first option, and some on the last

## Nuclear variational Monte Carlo method (Wiringa, Pandharipande, ...)

We wish to compute nuclear energy levels,  $S$ -matrix, etc. from a modern nuclear potential ( $\sim 20$  operator terms,  $\sim 30$  parameters, with 3-body terms)

The variational ansatz:

$$|\Psi_T\rangle = \left[ 1 + \sum_{i < j < k \leq A} U_{ijk}^{TNI} \right] \left[ \mathcal{S} \prod_{i < j \leq A} (1 + U_{ij}) \right] |\Psi_J\rangle$$

$$\begin{aligned} |\Psi_J\rangle = & \mathcal{A} \left\{ \prod_{i < j < k \leq 4} f_{ijk}^c \prod_{i < j \leq 4} f_{ss}(r_{ij}) \right. \\ & \times \sum_{LS[n]} \left( \beta_{LS[n]} \prod_{k \leq 4 < l \leq A} f_{sp}^{LS[n]}(r_{kl}) \right. \\ & \left. \left. \times \prod_{4 < l < m \leq A} f_{pp}^{LS[n]}(r_{lm}) |\Phi_A(LS[n]JMTT_z)_{1234:5\dots A}\rangle \right) \right\} \end{aligned}$$

Two-body correlations solve sets of differential equations built on the potential, three-body based on 1<sup>st</sup>-order perturbation

Each piece contains adjustable parameters, until recently optimized by hand into artisanal wave functions (now automated with adoption of Norfolk potentials)

## Drilling down farther

The VMC wave function is built from pieces of good  $L$ ,  $S$ ,  $J$ ,  $T$ , and Young diagram  $[n]$

E.g, for  ${}^6\text{Li}$

$$|\Phi_6(LS[n]JMTT_3)_{1234:56}\rangle = |\Phi_4(0000)_{1234}\phi_p^{LS[n]}(R_{\alpha 5})\phi_p^{LS[n]}(R_{\alpha 6}) \\ \times \left\{ [Y_{1m_i}(\Omega_{\alpha 5})Y_{1m'_i}(\Omega_{\alpha 6})]_{LM_L} \times [\chi_5(\frac{1}{2}m_s)\chi_6(\frac{1}{2}m'_s)]_{SM_S} \right\}_{JM} \times [\nu_5(\frac{1}{2}t_z)\nu_6(\frac{1}{2}t'_3)]_{TT_z}\rangle$$

As a final step after optimizing correlation parameters, amplitudes  $\beta_{LS[n]}$  of these things are found as a generalized eigenvalue problem

In  ${}^6\text{Li}$ , this means finding  $\beta_{01[42]}$ ,  $\beta_{10[411]}$ ,  $\beta_{21[42]}$

Long-range properties depend on what's built into the correlations

For scattering/reactions, we've focused on building the right asymptotics into the  $\phi_p^{LS[n]}$  at  $r \rightarrow \infty$

Other correlations either go to constants or decay rapidly (have to check that it's rapid enough)

These variational functions are often good approximations

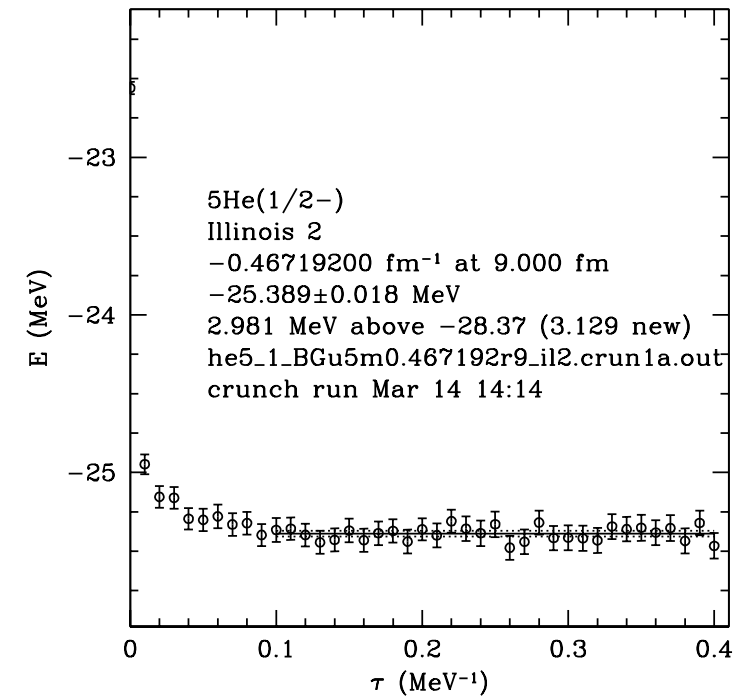
They do miss 1 MeV or more of binding (out of  $\sim 10$ ) per  $p$ -shell nucleon

## Nuclear Green's function Monte Carlo

We apply GFMC by diffusion in the coordinates,  
with importance sampling, & a propagator  
explicitly transforming spin/isospin vectors

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

$H$  is projected into “ $v'_8$  form” for propagator,  
remaining terms perturbative in  $\langle \Psi | \hat{H} | \Psi \rangle$

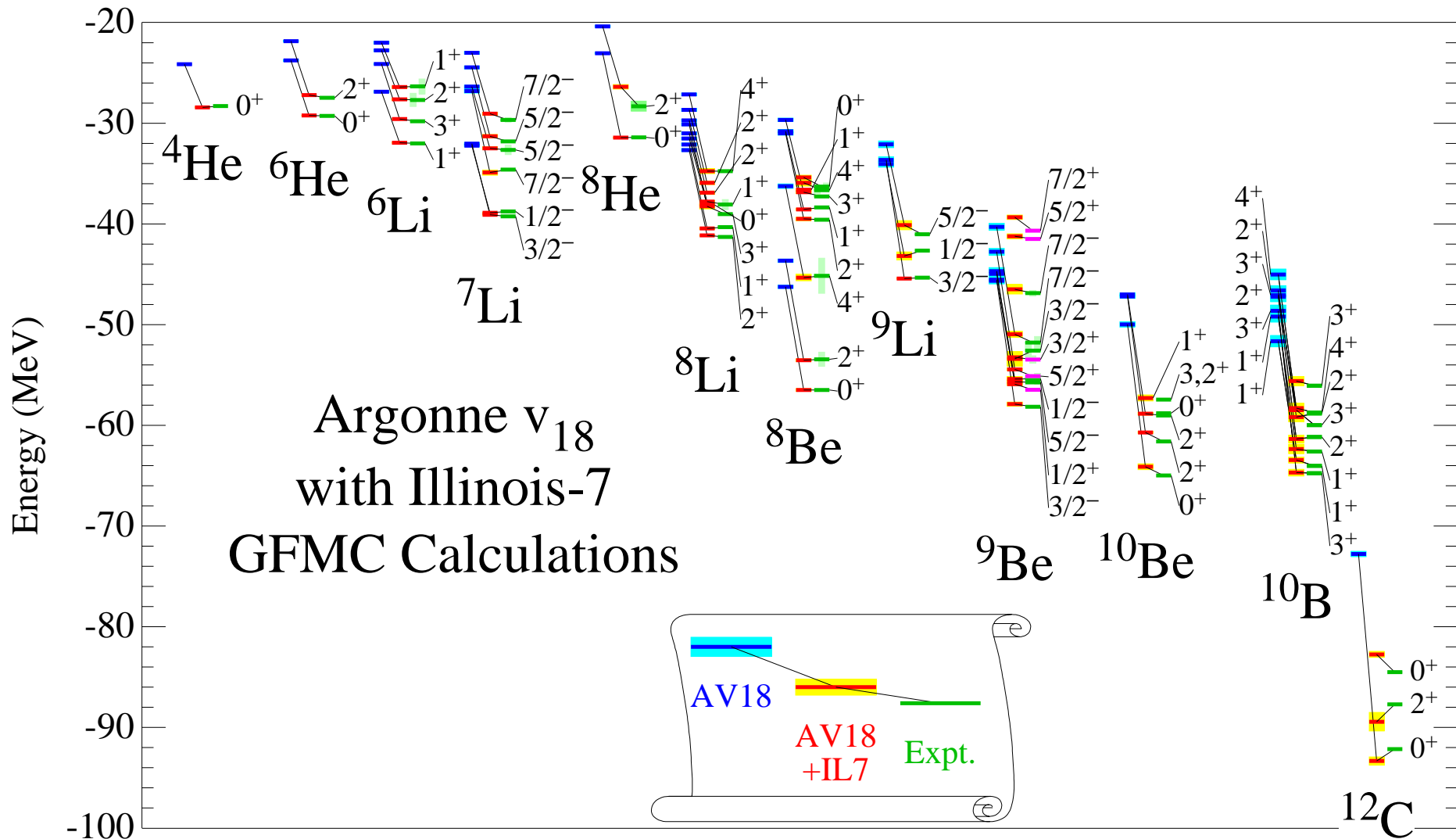


There is a path constraint based on avoiding sign changes in  $\text{Re}[\Psi(\mathbf{R})^\dagger \Psi_T(\mathbf{R})]$   
of spin-isospin vectors (simplifying a lot)

Walkers marked for killing are propagated an additional 20–80 steps first to  
remove bias

We believe that this gives lots of accurate energies up to  $A = 12$ , with statistical  
error & path constraint bias amounting to  $\sim 200$  keV





From review of Carlson et al. (2015)

Note that many of these are excitations of same  $J, T$ : eigensolutions of  $\beta_{LS}[n]$  amplitudes stay orthogonal in propagation

(Presumably  $\Psi_T^\dagger \Psi(\tau)$  sampling & path constraint do that)

## The outer limits

Reaction and scattering work requires more attention to the outer parts of  $\Psi(\tau)$  and  $\Psi_T$  than level energies

This is true even of bound states involved

In Nollett, Wiringa & Schiavilla (2001) and Nollett (2001), we looked at  $d(\alpha, \gamma)^6\text{Li}$ ,  $^3\text{H}(\alpha, \gamma)^7\text{Li}$ , and  $^3\text{He}(\alpha, \gamma)^7\text{Be}$  with VMC

We cheated on initial states – made them products of VMC projectiles, with a cluster-cluster correlation that reproduced phase shifts

But final bound states also needed correct tails, because at 10–500 keV that's where EM matrix elements come from for astrophysics

We built that into the  $\phi^{LS[n]}(r_{\alpha i})$   $p$ -shell orbitals with with correct clustering properties

## Single-channel scattering: the nodal boundary condition

Simplest single-channel scattering:

Set up an eigenvalue problem that maps onto scattering, minimize  $\langle E \rangle$  as before

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

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

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 to match de Broglie, & 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  $\gamma$ :

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

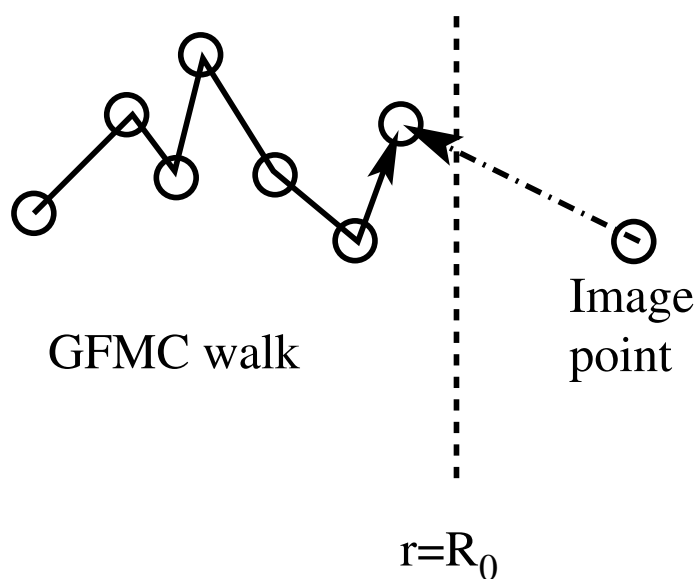
Then fix  $R_0$  at some “small” value (beyond nuclear radius and nucleon exchanges)

Vary the chosen  $\gamma$  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  $\phi_p^{LS[n]}$  radial orbitals in  ${}^5\text{He}$

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



In GFMC, we used a method of images from Carlson  
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  $\alpha n$  channel (must clip the  $\alpha$  a bit)

## Why ${}^5\text{He}$ scattering was painful

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

Scattering at  $E_{\alpha n} = 100$  keV requires  $0.100/28.3 = 0.3\%$  accuracy in  ${}^5\text{He}$  energy (and  ${}^4\text{He}$  energy, but that's easier to get)

At this level, dependence on the starting wave function  $\Psi_T$  was noticeable

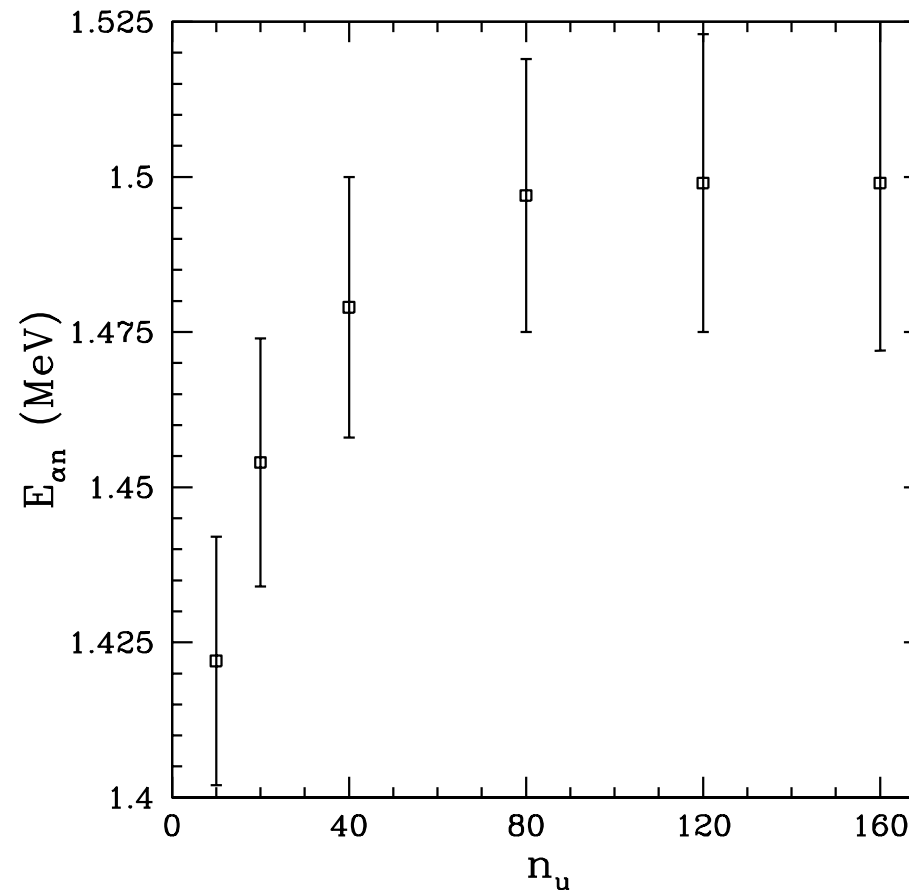
We eventually learned to cut off 2-body correlations beyond the size of  ${}^4\text{He}$

We also iterated (2 or 3 times) on single-particle energies in  $\Psi_T$  to tune the  ${}^4\text{He}+n$  starting wave function at large  $r_{\alpha n}$

We were also sensitive to the Monte Carlo path constraint

## Why ${}^5\text{He}$ was painful

In most(?)  $A \geq 5$  GFMC calculations, bias is reduced by removing the constraint for the final  $n_u = 10$  to 40 steps in  $\tau$  before an energy evaluation

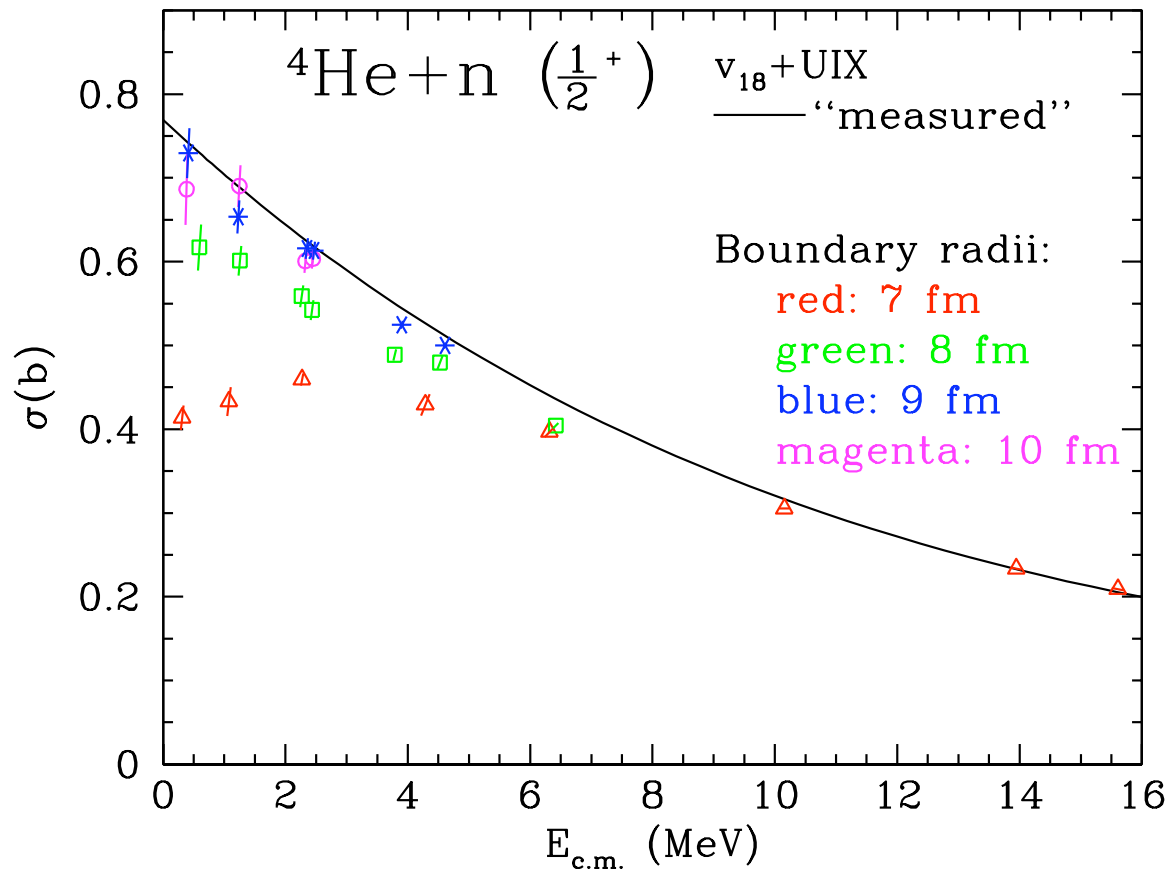


Maybe because the wave functions are more diffuse, we needed  $n_u \geq 80$  for smooth  $\delta(E)$  curves in  ${}^5\text{He}$

## Why ${}^5\text{He}$ was painful

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

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



$R = 7 \text{ fm}$  is not large enough

$R = 9 \text{ fm}$  is large enough

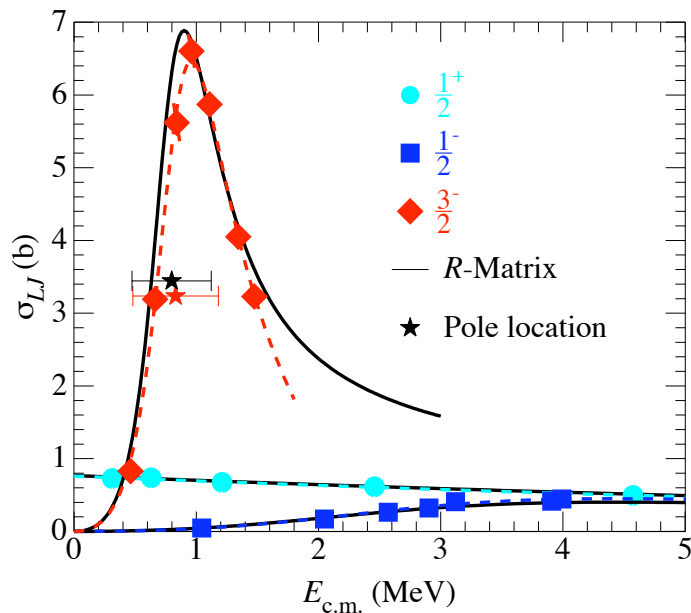
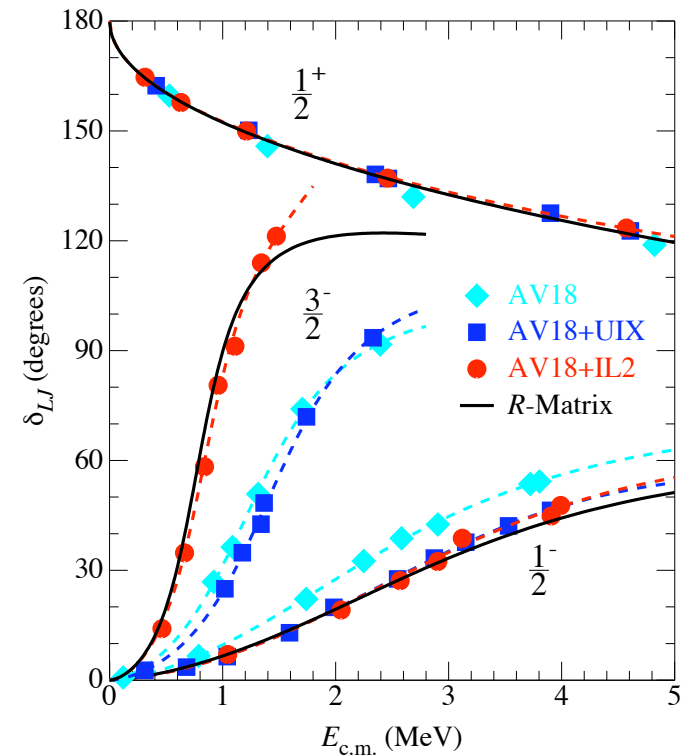


## Poles & scattering lengths

$s$ -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

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

This was repeated by Lynn et al. (2016) to fix  $NNN$  couplings in EFT potentials

## Some first attempts at $3 + 1$ scattering

$^5\text{He}$  was expected to be “easy” because there’s only one open channel,  $^4\text{He}$  is compact, scattering channel similar to VMC structure

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

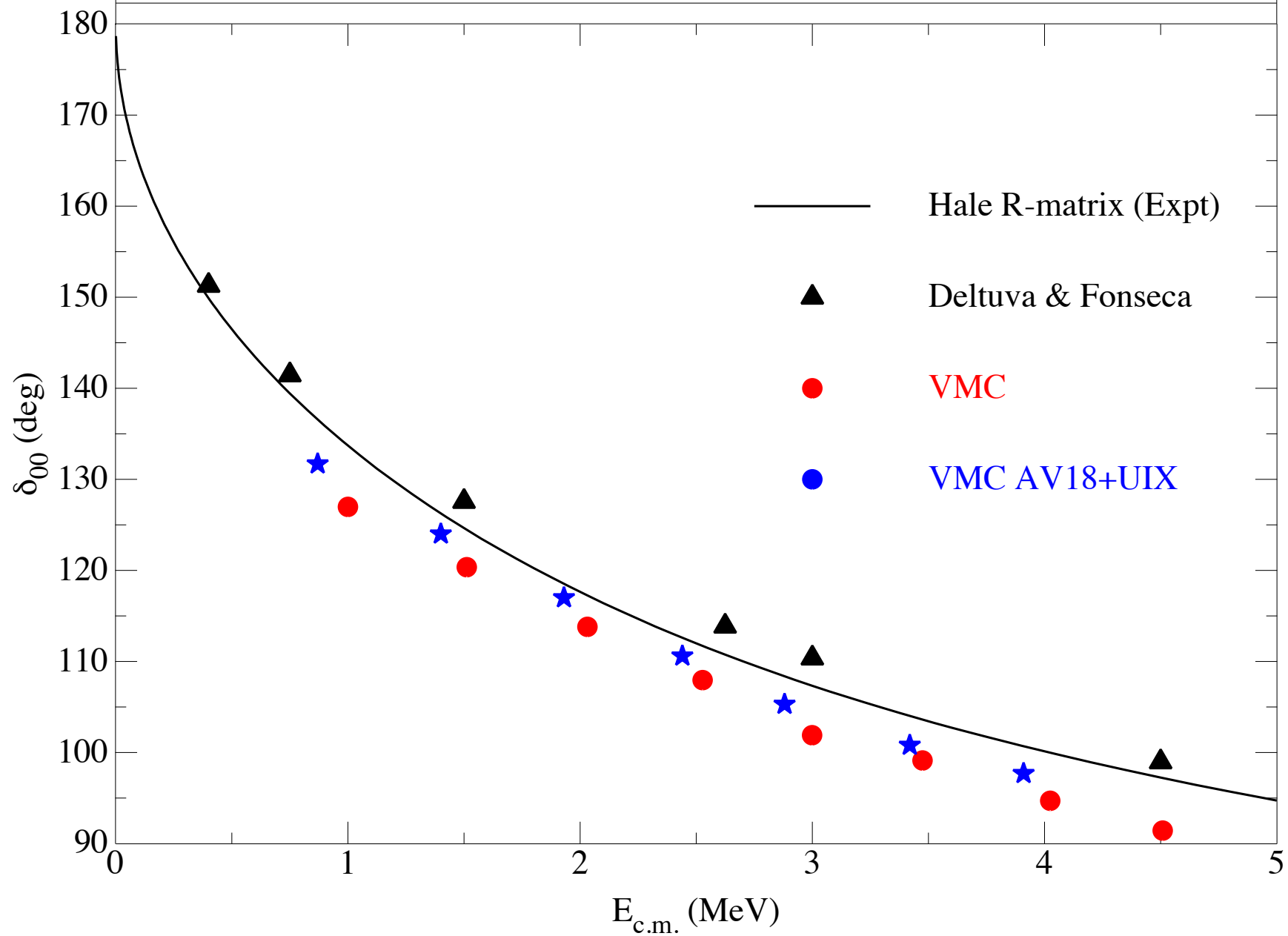
$A = 4$  would also allow a check against HH & AGS calculations

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

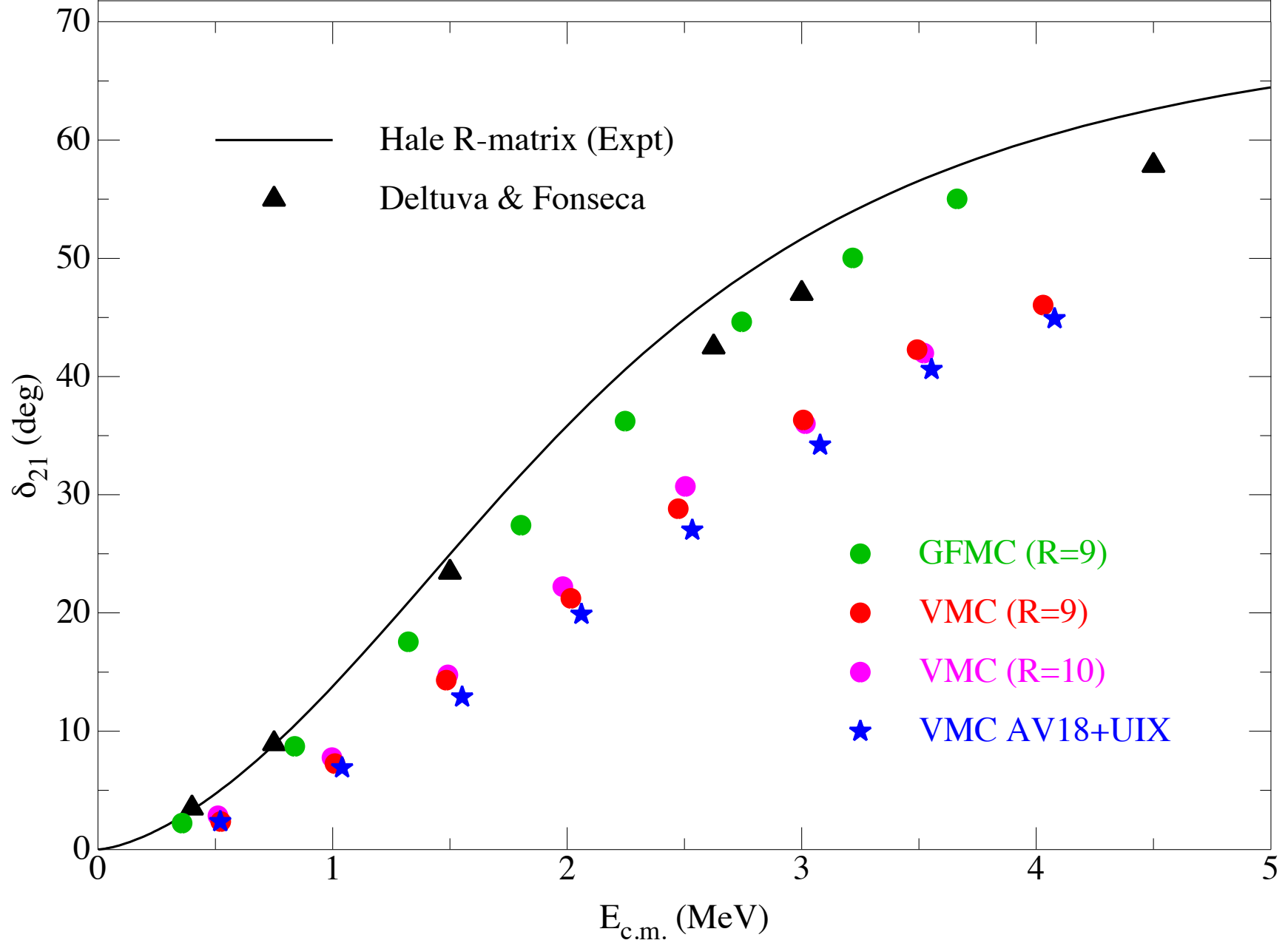
Breakup threshold is relatively high, no underlying bound states

Channel mixing is modest except in  $1^-$  channel

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

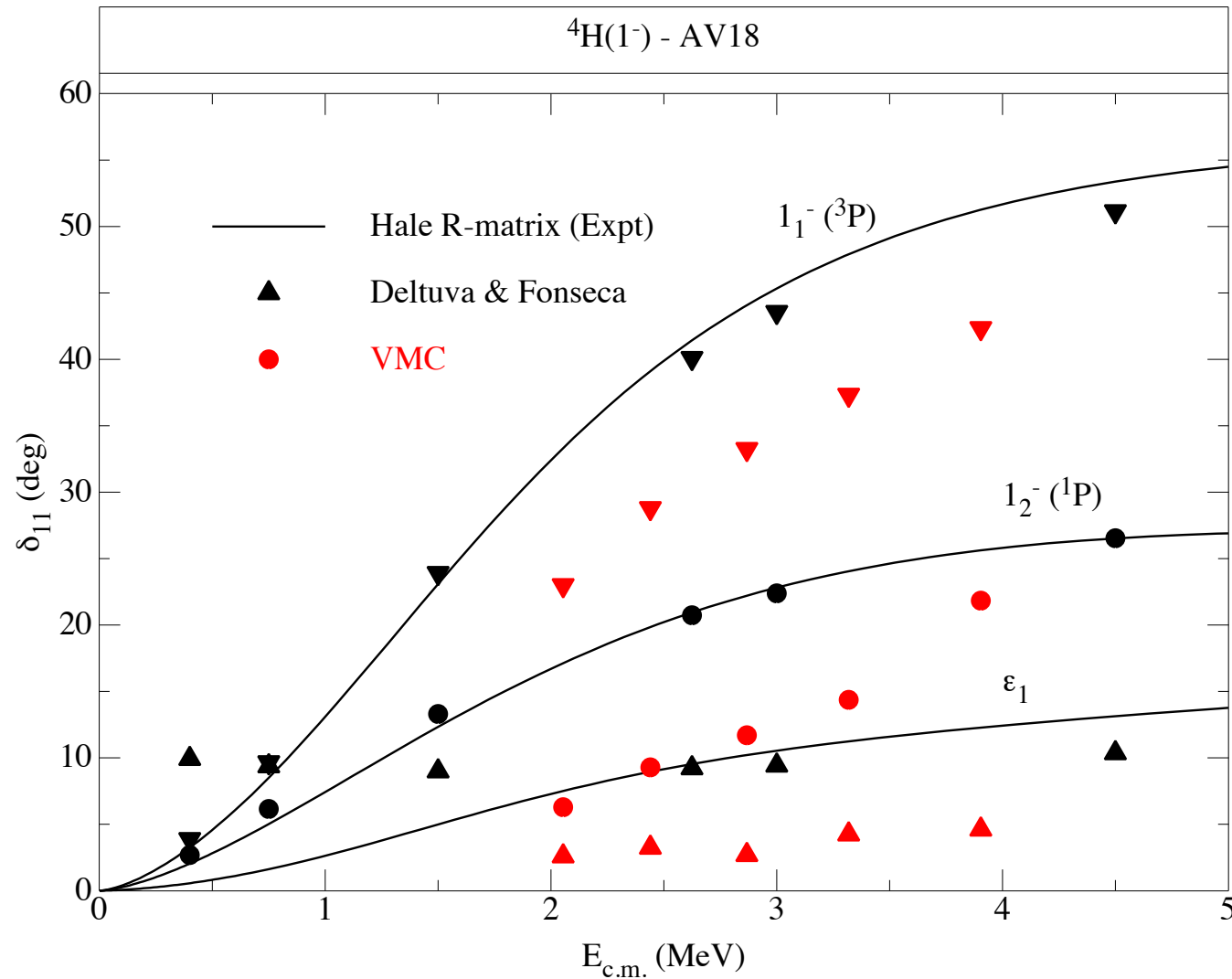
${}^4\text{H}(0^+) - \text{AV18}$ 

${}^4\text{H}(2^-) - \text{AV18}$



This one was easy to set up for GFMC

For  $1^-$  scattering, singlet & triplet channels mix, but we only made a start on coupled channels



At each energy, we computed two solutions, tried to extract  $S$ -matrix from  $\gamma$ 's & amplitudes at the channel radius

## The near future of VMC/GFMC scattering/reactions

I have a student starting on the  $3 + 1$  scatterings in  ${}^4\text{H}$  &  ${}^4\text{Li}$  now

We will check against accurate calculations with the same potentials (AV18+UIX to start, Norfolk later)

The main prize is to learn QMC coupled channels in a relatively gentle case: the  $1^-$  channels of  $S = 0$  and  $S = 1$  (& weaker tensor  $s$ - $d$  &  $p$ - $f$  couplings)

In the  $p$ -shell, there are few cases with only a one-nucleon channel open:  
 ${}^7\text{Be} + p, {}^7\text{Li} + n, \dots$

Those could be initial states for radiative capture & neutron spin rotation

A similar approach should work for  $\alpha + {}^3\text{H}, \alpha + {}^3\text{He}, \alpha + \alpha \dots$

But maybe need more-explicitly clusterized  $|\Phi\rangle$  functions in VMC for those

## Other ideas (not my current student)

The particle-in-a-box states are just the lowest in the tower of states used in  $R$ -matrix theory

We could in principle compute energies & surface amplitudes of lowest several, & get  $\delta(E)$  by insertion into  $R$ -matrix formalism

Ivan Brida started on the tower of states in  ${}^5\text{He}$  & had some promising early results

There is also a Lippmann-Schwinger-like formalism to generate correct tails from variational  $\Psi$  with the wrong tails

I've used it to extract tails of bound-state overlap functions (Nollett & Wiringa 2011) & rough estimates of nucleon emission widths (Nollett 2012)

It could be used for extraction of surface amplitudes in coupled channels VMC/GFMC, or for Born-like approximations to scattering

BONUS MATERIAL



## Thinking outside the box

Probably there are smarter things to be done than particle-in-a-box energy calculations

For GFMC, defining channels & finding surface amplitudes/derivatives is problematic (exchange effects, poor convergence, . . .)

(Amplitude is needed for wave function normalization and/or channel mixing)

I would also like to avoid getting surface amplitudes from surface values of the wave function – GFMC seems to converge slowly there

Lippmann-Schwinger-like approaches seem useful

## Integral relation for the ANC

There is a better way than explicit overlaps, ideally suited to QMC methods (appears in literature of 1960s, 1970s; this form from ~1990)

The Schrödinger equation

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

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

$$\Psi_A = - [T_{\text{rel}} + V_C + B]^{-1} (U_{\text{rel}} - V_C) \Psi_A$$

which implies

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

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

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

## Why is any of this useful?

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

The power of this approach lies in the factor  $(U_{\text{rel}} - V_C)$

It contains the potential, but only terms linking the core to the last particle:

$$U_{\text{rel}} = \sum_{i < A} v_{iA} + \sum_{i < j < A} V_{ijA}$$

At large separation of the last nucleon,  $U_{\text{rel}} \rightarrow V_C$ , so  $U_{\text{rel}} - V_C \rightarrow 0$

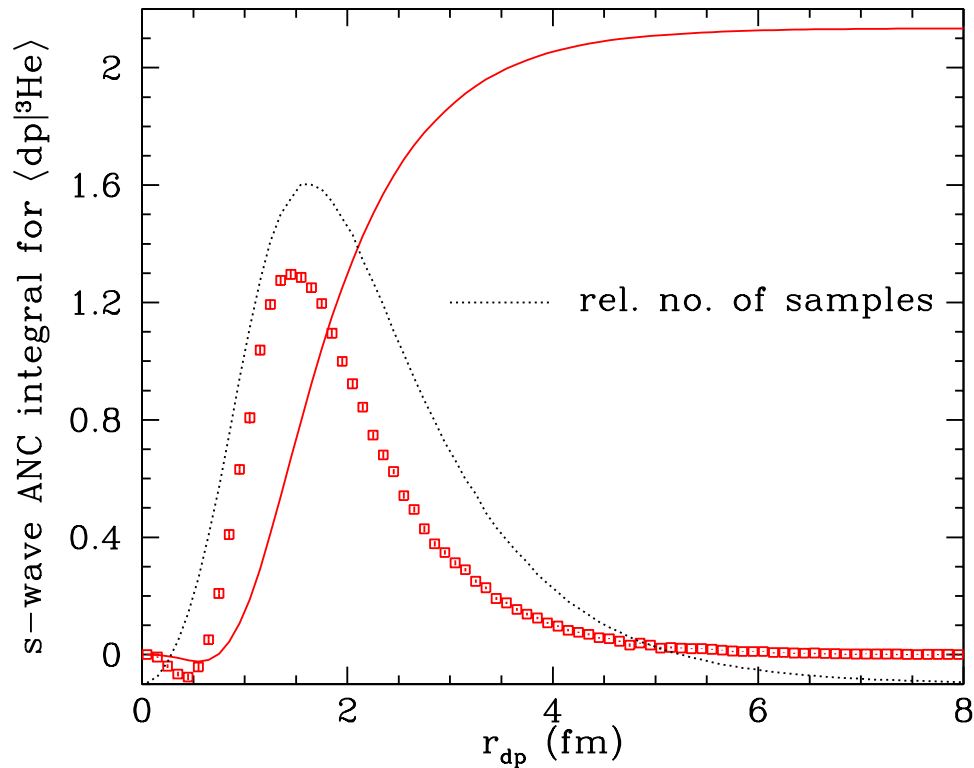
Integrand goes to zero at  $r_{cc} \sim 7$  fm with AV18+UIX

QMC methods are good at integration over the wave function interior, bad at the exterior

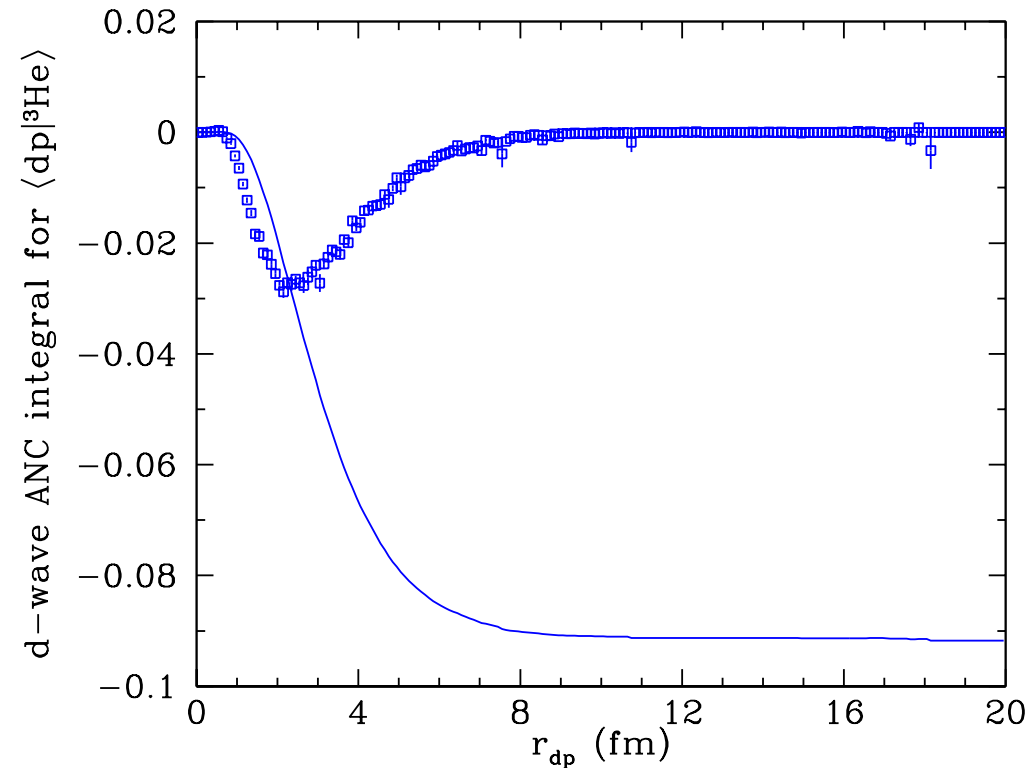
Closely related to Lippman-Schwinger equation (and to Pinkston-Satchler or Kawai-Yazaki overlaps); used by Mukhamedzhanov & Timofeyuk since  $\sim 1990$

## ANCs: ${}^3\text{He} \rightarrow dp$

### s-wave ANC integrand & integral



### d-wave ANC integrand & integral



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

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

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

## Application to the VMC wave functions

I implemented the integral approach to the ANC within the VMC code, building on Wiringa's spectroscopic factor routines

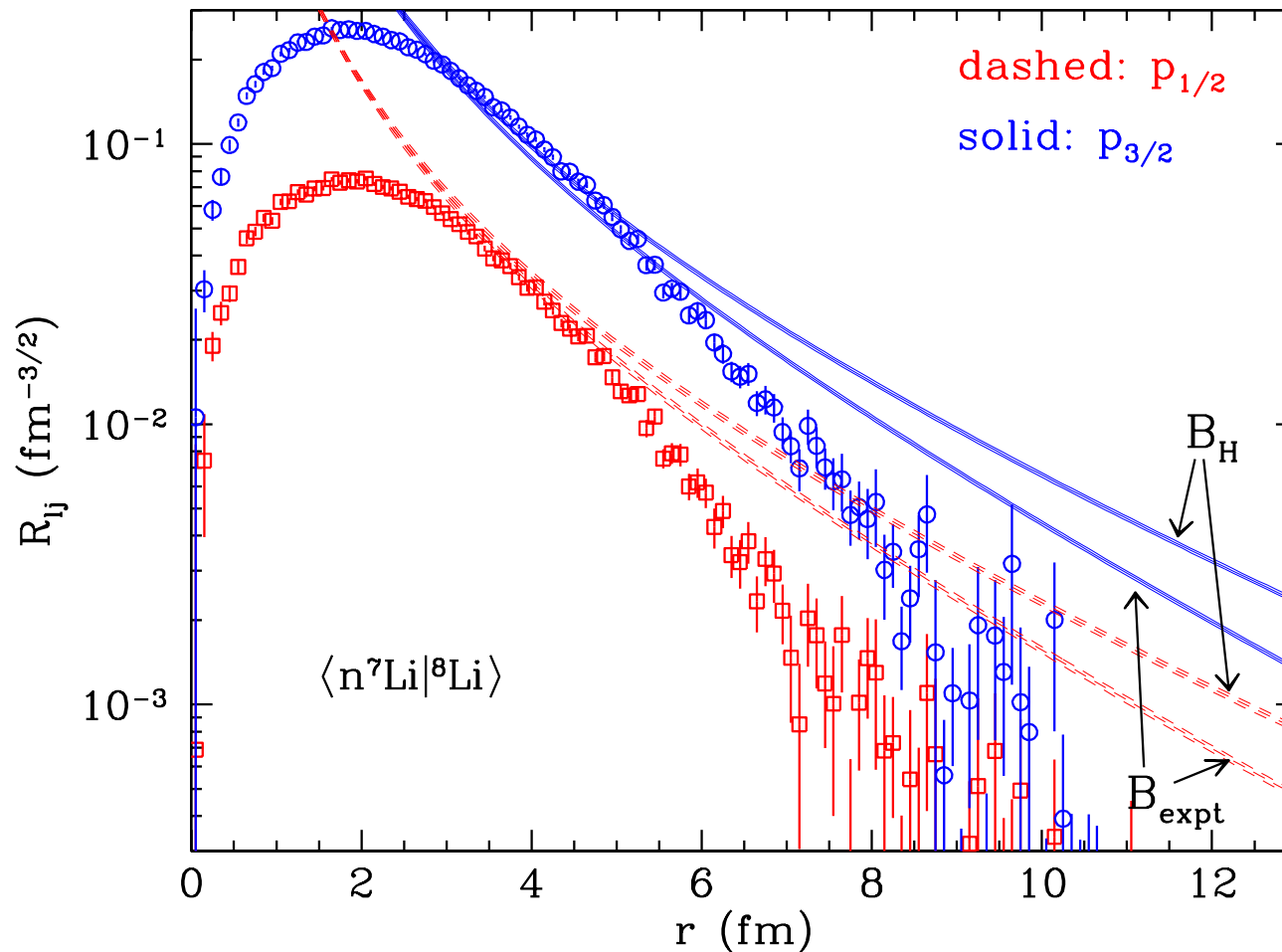
I computed ANCs from Bob's AV18+UIX VMC wave functions for almost every combination of particle stable  $A$ - and  $(A - 1)$ -body states at  $A \leq 9$

I have to choose a separation energy, either experimental or AV18+UIX, in evaluating each integral

It quickly became apparent that results match experiment only when the experimental separation energy is used

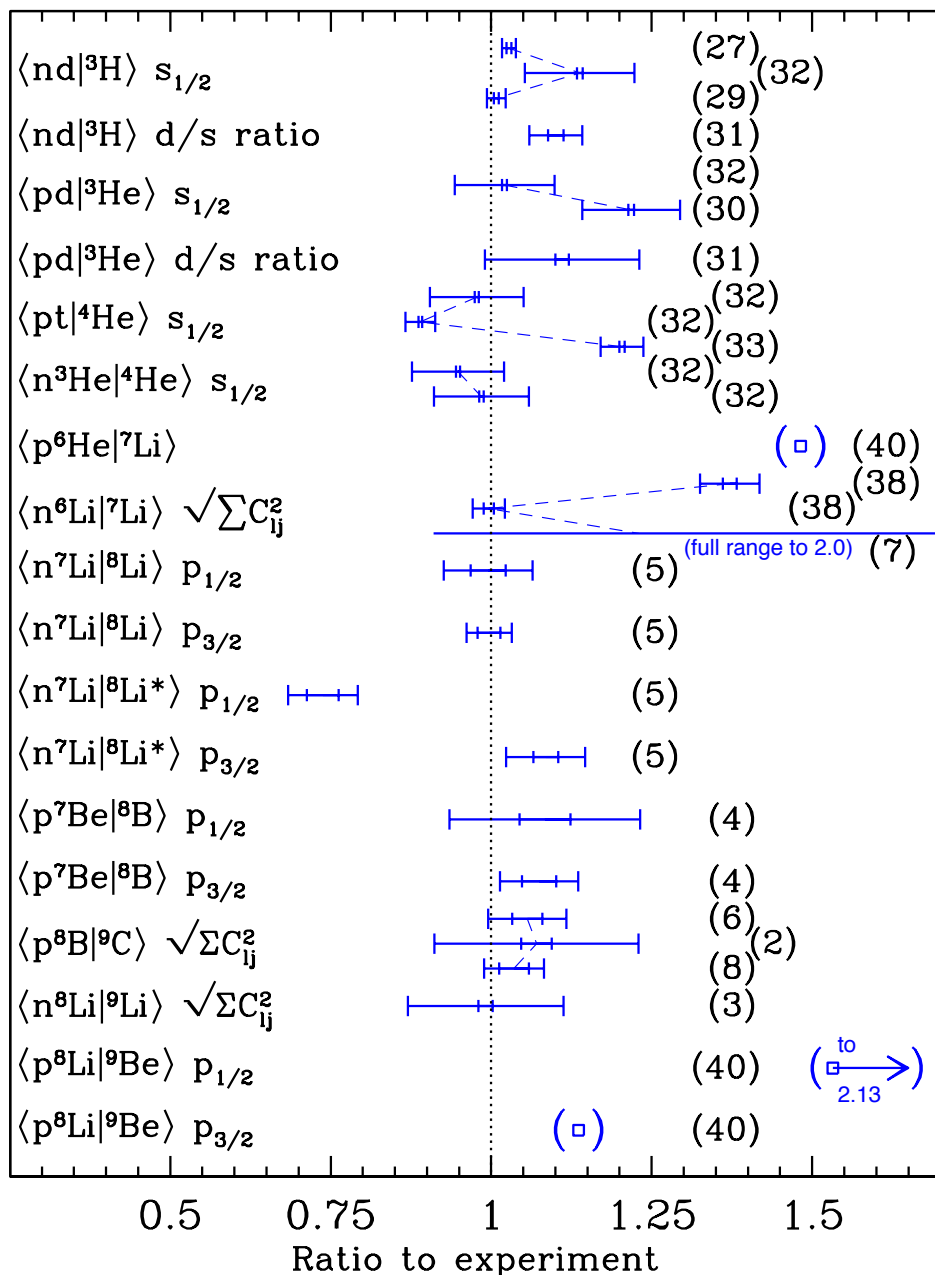
(Retrospective no-brainer: otherwise we're comparing against different functions)

${}^8\text{Li} \rightarrow {}^7\text{Li} + n$  summarizes the whole project



ANC ( $\text{fm}^{-1}$ )	VMC: AV18+UIX binding	VMC: Lab binding	Experiment
$C_{p1/2}^2$	0.029(2)	0.048(3)	0.048(6)
$C_{p3/2}^2$	0.237(9)	0.382(14)	0.384(38)

## Readable results, where there are “experimental” data



Small error bars are VMC statistics

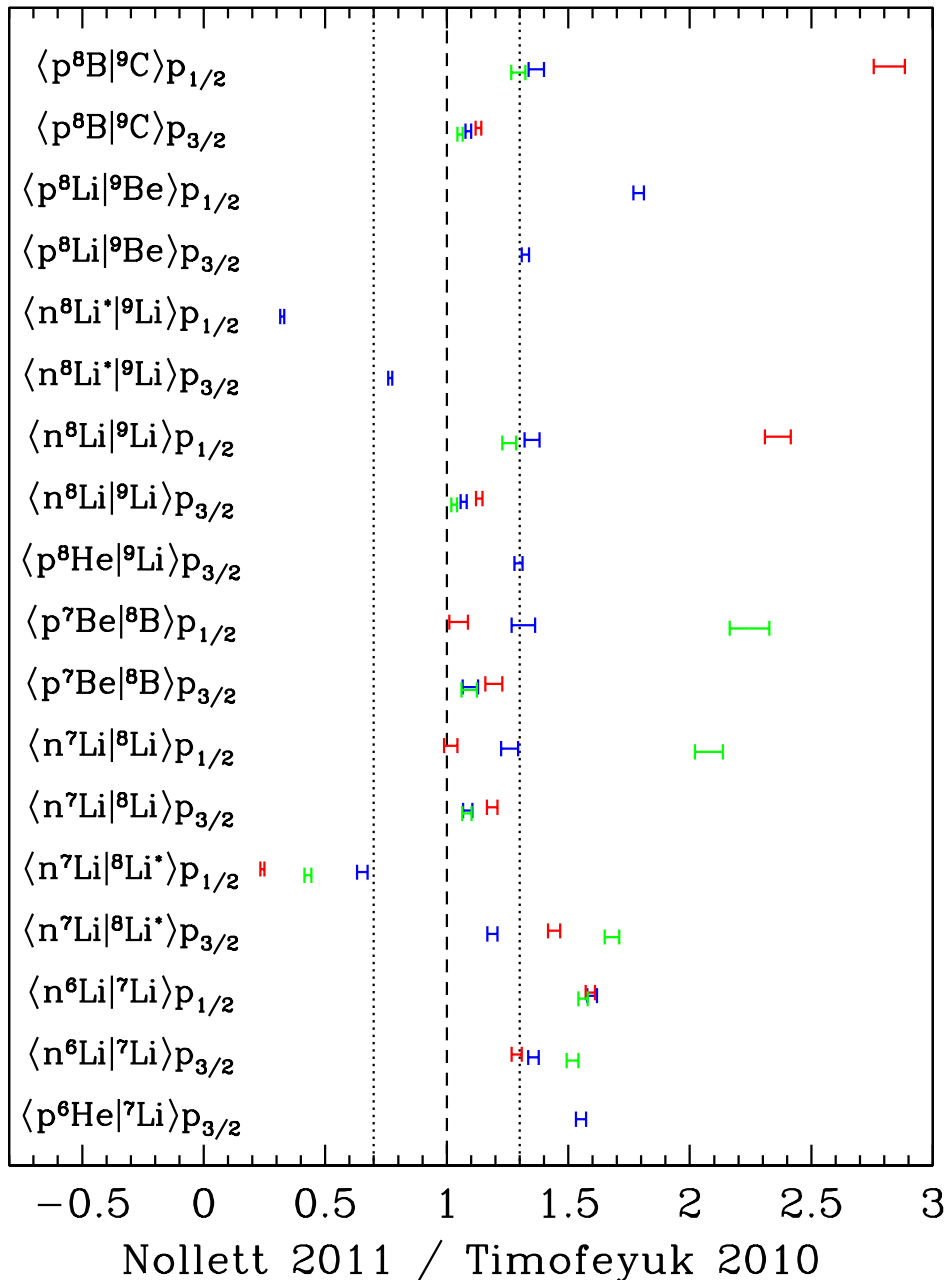
Large ones are “experimental”

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  $A > 4$

## Comparison with what came before



Timofeyuk has pursued a “hybrid” approach to the ANC integral for a long time

Wave functions come from p-shell model, integral from M3YE potential

Uncertainties have been hard to estimate

Colors denote shell model used in Timofeyuk 2010

Millener Boyarkina CK816

Attempts to derive ratios of isobaric-analogue ANCs from those calculations don't seem to hold up



## The results, $3 \leq A \leq 9$ one-nucleon removal

$A$	$A - 1$	$s_{1/2}$	$d_{3/2}$	$C_{d3/2}/C_{s1/2}$	
${}^3\text{H}$	${}^2\text{H}$	2.127(8)	-0.0979(9)	-0.0460(5)	
${}^3\text{He}$	${}^2\text{H}$	2.144(8)	-0.0927(10)	-0.0432(5)	
${}^4\text{He}$	${}^3\text{H}$	-6.55(2)			
${}^4\text{He}$	${}^3\text{He}$	6.42(2)			
$A$	$A - 1$	$p_{1/2}$	$p_{3/2}$	$f_{5/2} \times 10^3$	$f_{7/2} \times 10^3$
${}^7\text{Li}$	${}^6\text{He}$		3.68(5)		
${}^7\text{Li}^*$	${}^6\text{He}$	3.49(5)			
${}^7\text{Li}$	${}^6\text{Li}$	1.652(12)	1.890(13)	-78(20)	
${}^7\text{Li}^*$	${}^6\text{Li}$	-0.543(16)	-2.54(4)		
${}^7\text{Be}$	${}^6\text{Li}$	-1.87(3)	-2.15(3)	63(9)	
${}^7\text{Be}^*$	${}^6\text{Li}$	0.559(16)	2.59(5)		
${}^8\text{Li}$	${}^7\text{Li}$	0.218(6)	-0.618(11)	5.2(5)	2.5(15)
${}^8\text{Li}^*$	${}^7\text{Li}$	-0.090(3)	0.281(5)	-0.6(2)	
${}^8\text{B}$	${}^7\text{Be}$	0.246(9)	-0.691(17)	1.1(2)	-1.1(5)
${}^9\text{C}$	${}^8\text{B}$	-0.309(7)	1.125(12)	1.9(5)	-0.5(18)
${}^9\text{Li}$	${}^8\text{Li}$	0.308(7)	-1.140(13)	-4.1(10)	5(3)
${}^9\text{Li}$	${}^8\text{Li}^*$	-0.122(3)	0.695(7)	-1.1(6)	
${}^9\text{Li}$	${}^8\text{He}$		-5.99(8)		
${}^9\text{Be}$	${}^8\text{Li}$	5.03(6)	9.50(11)	35(34)	257(112)
${}^9\text{Be}$	${}^8\text{Li}^*$	6.56(5)	-6.21(7)	364(40)	

Nollett & Wiringa, PRC 83, 041001(R) (2011)

The small  $f$ -wave amplitudes are accessible with this method – unknown how reliable (or measurable), but something new

## Heights and widths



“The other day I was walking my dog around my building, on the ledge. Some people are afraid of heights. I’m afraid of widths.”

– Steven Wright

We have VMC/GFMC energies for many narrow unbound levels (computed as bound)

Figuring out how to get widths has been difficult

There is an obvious but laborious way – explicit calculation of phase shifts at many energies, extraction of pole (has been done for  $^5\text{He}$  states)

Other paths have not panned out (e.g. “decay” rate in GFMC)

## Widths as ANCs

Widths are closely related to ANCs, so maybe there's a cheap way to estimate them

Hand-waving description:

An unbound wave function at large radius looks like

$$\psi(r \rightarrow \infty) \propto [F_l(kr) \cos \delta + G_l(kr) \sin \delta] / r$$

so that at resonance ( $\delta = 90^\circ$ ; as our pseudobound states should have)

$$\psi(r \rightarrow \infty) = C_{lj} \phi_1 \phi_2 G_l(kr) / r$$

The flux per unit time through the surface is  $|C_{lj}|^2 v = \frac{\hbar k}{\mu} |C_{lj}|^2$ , so

$$\Gamma \simeq \frac{\hbar^2 k}{\mu} |C_{lj}|^2$$

This is to be shown to be nearly exact in papers by Humblet (not by this reasoning)

## Widths as ANCs

The relation

$$\psi(r \rightarrow \infty) = C_{lj} \phi_1 \phi_2 G_l(\eta, kr) / r$$

for resonant states is mathematically almost the same as

$$\psi(r \rightarrow \infty) = C_{lj} \phi_1 \phi_2 W_{-\eta, l + \frac{1}{2}}(2kr) / r$$

for bound states

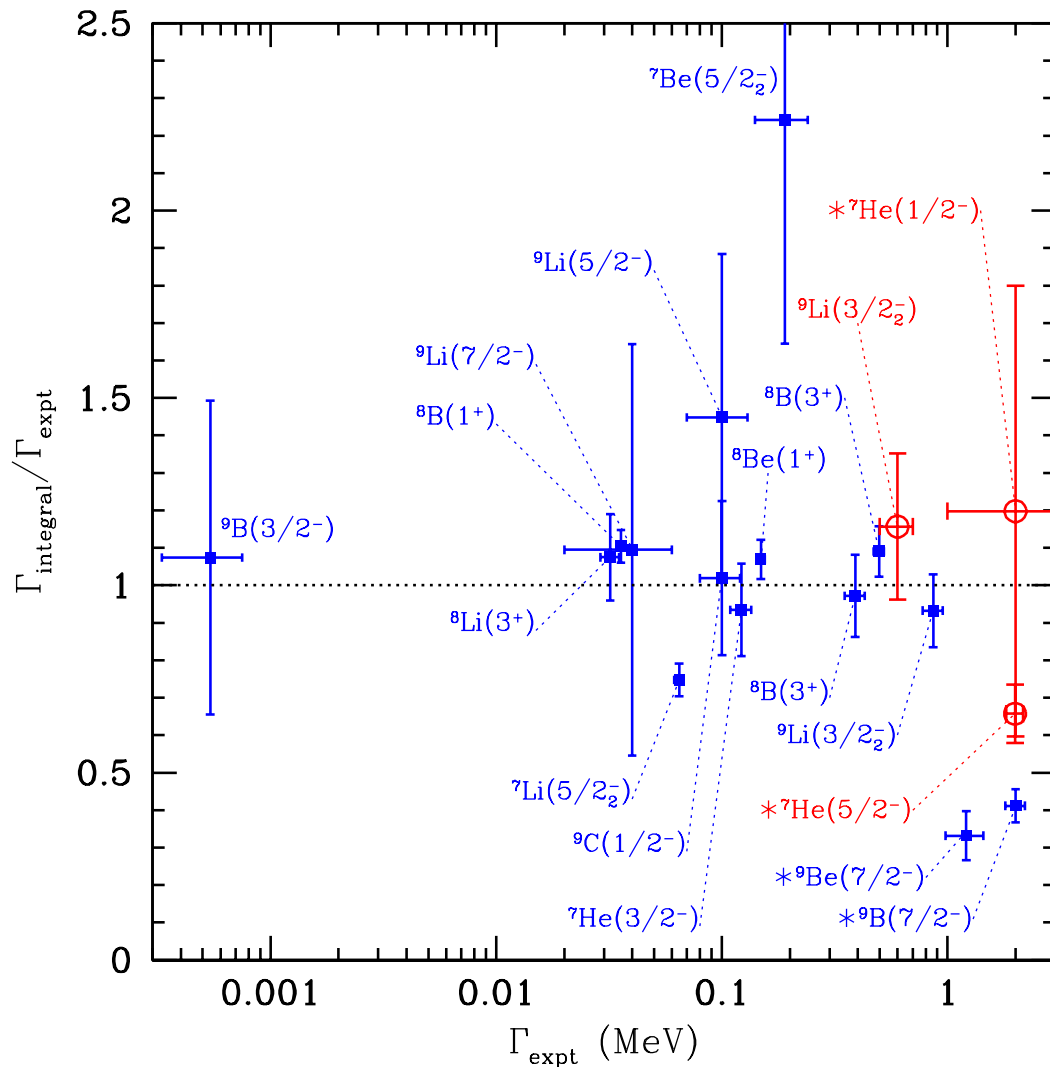
The integral method also applies to resonant states, except that now  $F_l$  appears in the integral instead of  $M_{-\eta, l + \frac{1}{2}}$

This is used as a mathematical tool to get the asymptotics right in simpler  $\alpha$  and  $p$  decay models (e.g. Åberg et al. (1997) proton emitters, Russian literature on  $\alpha$  decay, etc.)

## Testing out the integral relation for $\Gamma$

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

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

# Testing out the integral relation for $\Gamma$

I computed a pretty complete set of these

State	Daughter	Experiment		From Exp energy		From AV18+UIX energy		Matches 90°?	$\zeta$
		$E$ (MeV)	$\Gamma$ (MeV)	$\Gamma_{VMC}$ (MeV)	$E_{UIX}$ (MeV)	$\Gamma_{VMC}$ (MeV)			
$^5\text{He}(3/2^-)$	$^4\text{He}(0^+)$	0.798	0.648 [50]	0.307(5)	1.39	0.684(11)	no	0.460	
$^5\text{He}(1/2^-)$	$^4\text{He}(0^+)$	2.07	5.57 [50]	0.582(13)	2.4	0.711(15)	no	0.429	
$^7\text{He}(3/2^-)$	$^6\text{He}(0^+)$	0.445	0.15(2)	0.114(4)	2.3	1.184(9)	yes	0.092	
$^7\text{He}(1/2^-)$	$^6\text{He}(0^+)$	3.045	–	1.98(9)	2.91	1.87(8)	no	0.092	
$^7\text{He}(1/2^-)$	$^6\text{He}(2^+)$	1.25	–	0.42(3)	1.11	0.36(2)	yes	0.067	
$^7\text{He}(1/2^-)$	sum	3.045	2.0(1.0)	2.40(12) <sup>a</sup>	2.91	2.22(11) <sup>a</sup>			
$^6\text{He}(5/2^-)$	$^6\text{He}(2^+)$	1.57	1.99(17)	1.31(10) <sup>a</sup>	1.87	1.66(13) <sup>a</sup>	no	0.165	
$^7\text{Li}(5/2_2^-)$	$^6\text{Li}(1^+)$	0.204	0.0646	0.0483(17) <sup>a</sup>	1.55	0.92(3) <sup>a</sup>	yes	0.055	
$^7\text{Be}(5/2_2^-)$	$^6\text{Li}(1^+)$	1.60	0.19(5)	0.426(14) <sup>a</sup>	2.5	1.00(3) <sup>a</sup>	yes	0.055	
$^8\text{B}(1^+)$	$^7\text{Be}(3/2^-)$	0.632	–	0.0383(14)	1.47	0.346(12)	yes	0.001	
$^8\text{B}(1^+)$	$^7\text{Be}(1/2^-)$	0.203	–	0.00105(6)	1.38	0.51(3)	yes	0.003	
$^8\text{B}(1^+)$	sum		0.0357(6)	0.0394(14)		0.86(3)	yes		
$^8\text{Li}(3^+)$	$^7\text{Li}(3/2^-)$	0.223	0.032(3)	0.0344(18)	2.5	1.12(6)	yes	0.007	
$^8\text{B}(3^+)$	$^7\text{Be}(3/2^-)$	2.18	0.39(4)	0.38(2)	2.4	0.46(2)	yes	0.007	
$^8\text{B}(0^+)$	$^7\text{Be}(3/2^-)$	[2.56]	–	[0.65(4)]	2.39	0.57(3)	no	0.005	
$^8\text{B}(0^+)$	$^7\text{Be}(1/2^-)$	[2.24]	–	[1.23(6)]	2.30	1.29(7)	no	0.004	
$^8\text{Li}(0^+)$	$^7\text{Li}(3/2^-)$	[0.97]	–	[0.37(2)]	0.94	0.389(15)	no	0.005	
$^8\text{Li}(0^+)$	$^7\text{Li}(1/2^-)$	[0.62]	–	[0.516(18)]	0.62	0.72(2)	no	0.004	
$^8\text{Be}(1^+) T = 1^b$	$^7\text{Li}(3/2^-)$	0.385	–	0.0089(3)	1.2	0.152(3)	yes	0.003	
$^8\text{Be}(1^+) T = 0^b$	$^7\text{Li}(3/2^-)$	0.895	–	0.150(4)	0.5	0.0354(10)	yes	0.003	
$^8\text{Be}(1^+) \text{sum}^b$	$^7\text{Li}(3/2^-)$		0.149(6)	0.159(4)		0.187(3)	yes		
$^8\text{Be}(3^+) T = 1^b$	$^7\text{Li}(3/2^-)$	1.81	–	0.166(8)	3.68	0.60(3)	yes	0.007	
$^8\text{Be}(3^+) T = 0^b$	$^7\text{Li}(3/2^-)$	1.98	–	0.314(14)	2.33	0.43(2)	yes	0.003	
$^8\text{Be}(3^+) T = 1^b$	$^7\text{Be}(3/2^-)$	0.170	–	0.0115(6)	2.09	0.44(2)	yes	0.007	
$^8\text{Be}(3^+) T = 0^b$	$^7\text{Be}(3/2^-)$	0.335	–	0.050(2)	0.74	0.161(8)	yes	0.004	
$^8\text{Be}(3^+) \text{sum}^b$	sum		0.50(3)	0.542(16)		1.63(4)	yes		
$^9\text{Li}(5/2^-)$	$^8\text{Li}(2^+)$	0.232	0.10(3)	0.145(4)	0.97	1.17(3)	yes	0.003	
$^9\text{Li}(7/2^-)$	$^8\text{Li}(2^+)$	2.366	–	0.0012(7)	3.64	0.0031(16)	no	0.045	
$^9\text{Li}(7/2^-)$	$^8\text{Li}(3^+)$	0.111	–	0.0427(8)	0.23	0.126(3)	yes	0.006	
$^9\text{Li}(7/2^-)$	sum		0.04(2)	0.0439(11)		0.129(3)			
$^9\text{Li}(3/2_2^-)$	$^8\text{Li}(2^+)$	1.316	–	0.522(13)	1.51	0.631(17)	no	0.014	
$^9\text{Li}(3/2_2^-)$	$^8\text{Li}(1^+)$	0.340	–	0.172(4)	0.50	0.302(8)	yes	0.006	
$^9\text{Li}(3/2_2^-)$	sum		0.6(1)	0.694(18)		0.932(19)			
$^9\text{C}(1/2^-)$	$^8\text{B}(2^+)$	0.918	0.10(2)	0.102(3)	1.54	0.428(11)	yes	0.006	
$^9\text{Be}(1/2^-)$	$^8\text{Be}(0^+)$	1.110	0.86(9)	0.80(2)	4.37	4.89(12)	yes	0.0005	
$^9\text{B}(3/2^-)$	$^8\text{Be}(0^+)$	0.185	0.00054(21)	0.00058(2)	1.9	0.92(2)	yes	0.0003	
$^9\text{Be}(7/2^-)$	$^8\text{Be}(0^+)$	4.715	–	0.0082(4)	–	–	yes	0.005	
$^9\text{Be}(7/2^-)$	$^8\text{Be}(2^+)$	1.685	–	0.40(2)	–	–	yes	0.003	
$^9\text{Be}(7/2^-)$	sum		1.2(2)	0.41(2) <sup>a</sup>	–	–	yes		
$^9\text{B}(7/2^-)$	$^8\text{Be}(2^+)$	4.13	2.0(2)	0.82(4) <sup>a</sup>	–	–	yes	0.003	
$^8\text{B}(2_2^+)$	$^7\text{Be}(3/2^-)$	2.41	0.12(4)	0.425(15)	–	–	yes	0.004	
$^8\text{B}(2_2^+)$	$^7\text{Be}(1/2^-)$	1.98	0.24(11)	0.039(2)	–	–	yes	0.010	
$^8\text{Li}(2_2^+)$	$^7\text{Li}(3/2^-)$	[2.18]	–	[1.00(4)]	–	–	yes	0.004	
$^8\text{Li}(2_2^+)$	$^7\text{Li}(1/2^-)$	[2.06]	–	[0.105(6)]	–	–	yes	0.010	

Some work, some don't

But this is useful practice for  
more serious calculations

## Overlaps at all radii

The ANC/width integrals are special cases of the overlaps of Pinkston & Satchler (or Kawai & Yazaki):

$$R_{lj}(r) \propto \left[ \cos \delta_{lj} + \int_r^\infty \frac{G_l(kr_{cc})}{r_{cc}} \Psi_{A-1}^\dagger \chi^\dagger(U_{\text{rel}} - V_C) \Psi_A d\mathbf{R} \right] F_l(kr)/r \\ + \left[ \int_0^r \frac{F_l(kr_{cc})}{r_{cc}} \Psi_{A-1}^\dagger \chi^\dagger(U_{\text{rel}} - V_C) \Psi_A d\mathbf{R} \right] G_l(kr)/r$$

90° phase shift means no  $F_l$  component at  $r \rightarrow \infty$

If this  $R_{lj}$  with  $\cos \delta_{lj} = 0$  is a poor match to the directly-computed overlap at small  $r$ , then  $\delta \neq 90^\circ$  for that channel  $\rightarrow$  my assumptions are invalid

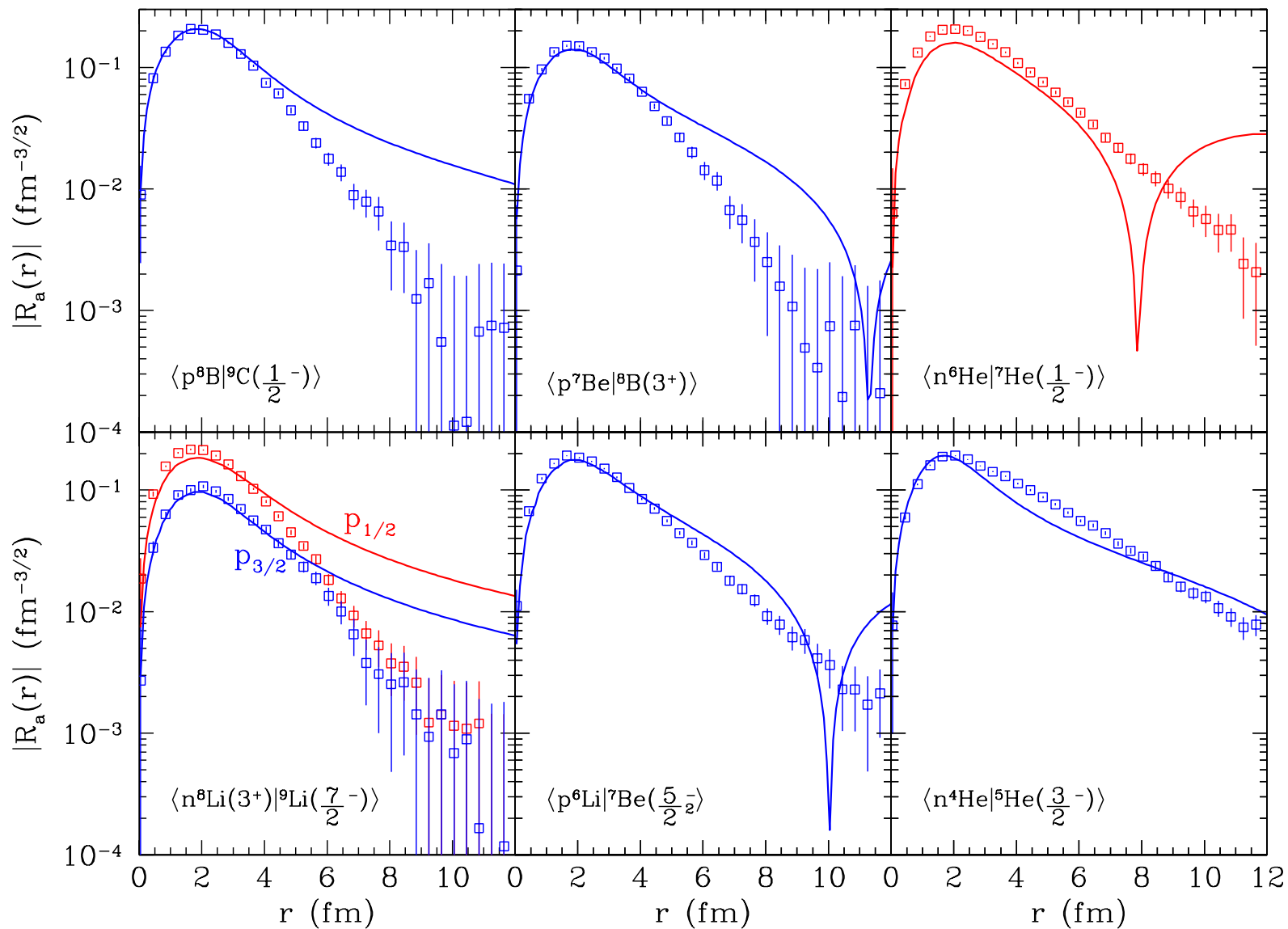
Cases that fail this test generally have small spectroscopic factors

# Overlaps at all radii

Good

Good

Bad



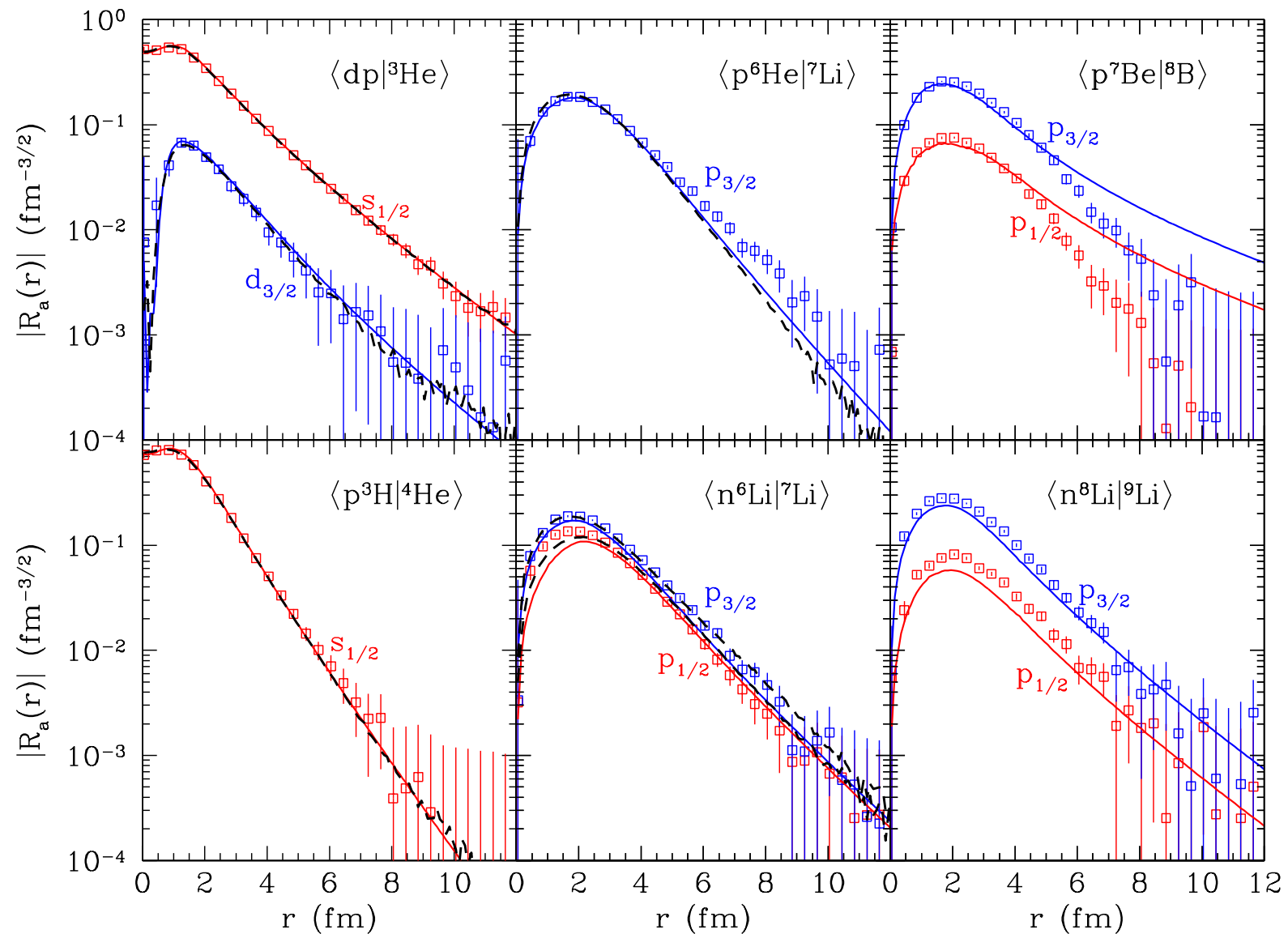
Points: Direct overlap

Curves: From integral relation



## Overlaps at all radii: Bound states

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



## What next? (no particular order)

Repeat for  $\alpha$  removal/decay instead of nucleon removal

Examining failure of Timofeyuk isospin-symmetry argument in  ${}^7\text{Be}/{}^7\text{Li}$   
(Isospin-breaking terms in AV18?)

GFMC & better potentials for better comparison with experiment

It would be interesting to do some honest scattering calculations for states where pseudobound is “successful”

That requires a “Goldilocks state:” not too wide for pseudobound, not too narrow for GFMC to map phase shifts

## What next? (no particular order)

Pseudobound approaches to  $\delta(E)$  (Horiuchi et al., Kievsky et al., etc.) might be well suited to VMC – worth a try!

Set up a resonant or low-lying nonresonant state as a bound-state calculation like we usually do

Then scan over energies in the integral-relation “kernels” to map phase shifts

That might be good for treatment of finite width in EW transitions

Integral methods are probably the best way to define channels through “left-side” wave function & get surface amplitudes from GFMC

Energy resolutions below the 100 keV range are difficult for GFMC, so the integral approach will beat phase-shift mapping for really narrow states

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