Ab initio nuclear widths, real and virtual

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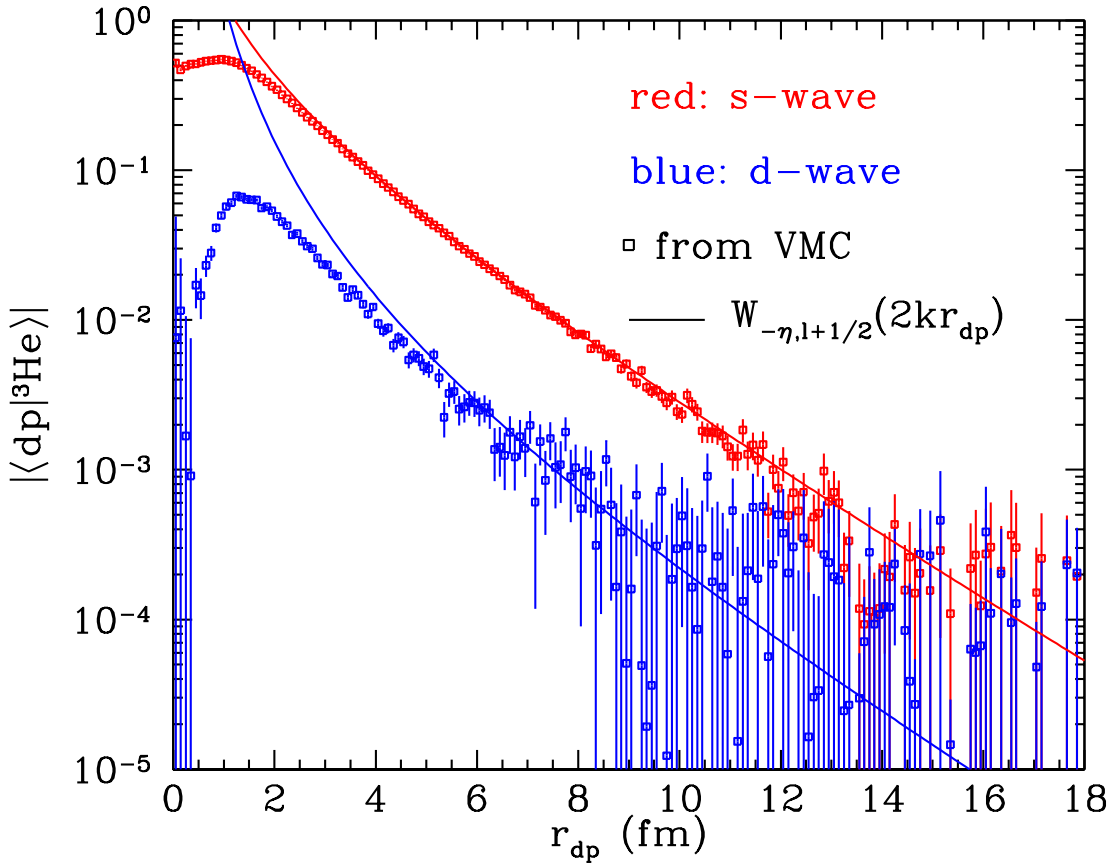
Nollett & Wiringa, PRC 83, 041001(R) (2011), and in preparation

Asymptotic normalization coefficient (ANC): definition

Many-body wave functions at large cluster separations factorize into clusters times a known shape:

$$\Phi_{^3\mathrm{He}}(r_{pd} \to \infty) = \sum_{l=0,2} C_{lj}\phi_d\phi_p Y_{lm}(\hat{\mathbf{r}}_{pd}) W_{-\eta,l+\frac{1}{2}}(2kr_{pd})/r_{pd}$$



At long range, nuclear dynamics just set E ($\to \eta, k$) and C_{lj}

Relation between ANCs and observables

Clearest case is low-energy direct capture, $X + Y \longrightarrow Z + \gamma$

At E well below the Coulomb barrier, the initial-state wave function has very small amplitude in the nuclear interior (has to tunnel), large r dominates matrix element, $\sigma \propto C_{lj}^2$

Bound states produce negative-energy poles in the scattering amplitude $\longrightarrow$ ANCs $\propto$ residues and can sometimes be extracted from analytically-continued scattering data (1970s)

Most ANC determinations (usually motivated by capture) came from transfer, knockout, or breakup reactions

These are special cases of "spectroscopic factor" experiments, requiring demonstrated independence from small-r contributions

ANCs in transfer reactions

ANC or spectroscopic factor experiments are meant to probe the cluster overlap function

$$R_{lj}^{J_{A-1}J_A}(r) \equiv \int \mathcal{A}\left[\Psi_{A-1}^{J_{A-1}}\left[\chi Y_l(\hat{\mathbf{r}})\right]_j\right]_{J_A}^{\dagger} \frac{\delta(r-r_{cc})}{r^2}\Psi_A^{J_A}\, d\mathbf{R}$$

and particularly

$$S_{lj} \equiv \int R_{lj}^2(r) r^2 dr$$

cf. Furnstahl's slides from last week for limitations and ambiguities of S_{lj}

Since $R_{lj}(r \to \infty) = C_{lj} W_{-\eta,l+\frac{1}{2}}(2kr)/r$, the ANC C_{lj} can in principle be isolated in data restricted to large impact parameter

Some of the usual limitations (e.g. optical potentials) apply just as well to C_{lj} as to S_{lj}

Consistency of R_{lj} between reaction & structure theory is easier for C_{lj} than for S_{lj}, provided that you can prove peripherality

Why I was motivated to compute ANCs

Should be useful for astrophysics

Relatively few ANCs have been measured $\longrightarrow$ an opportunity for pre- rather than post-diction

ANCs can be computed from *ab initio* wave functions, but accurate results are a challenge (reasons will follow)

ANCs provide a learning problem for computational techniques needed for scattering/reaction problems

Why quantum Monte Carlo ANCs require effort

GFMC requires all the work of variational Monte Carlo plus more, so for now I work with VMC wave functions:

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

Each piece contains variational parameters, found by minimizing energy as computed by Monte Carlo integration

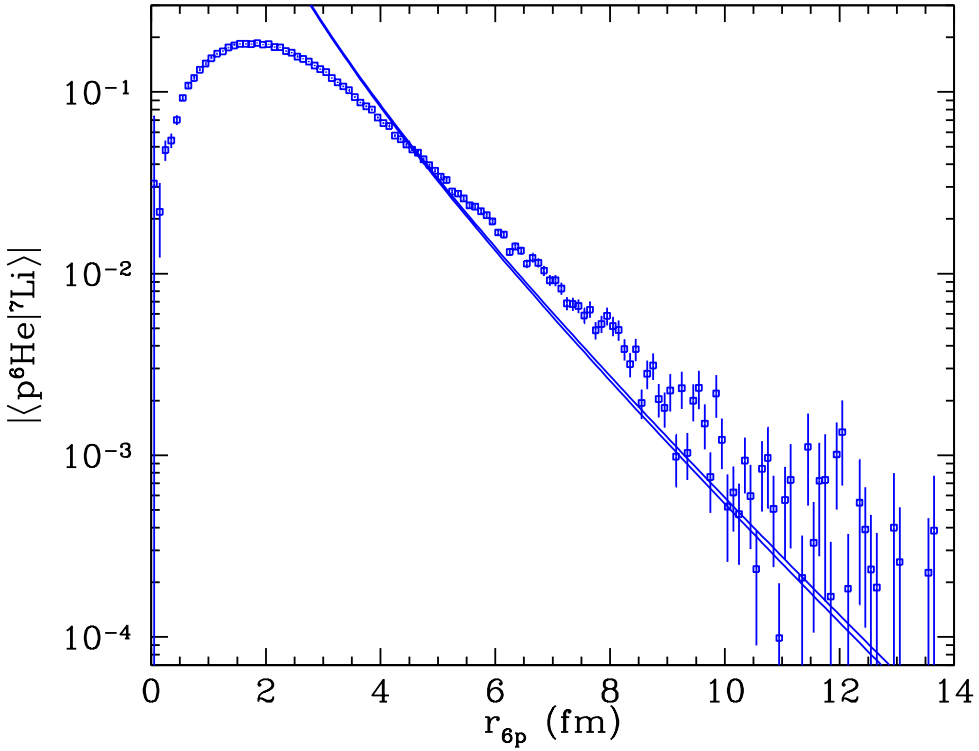
The VMC ansatz is very good and allows rather accurate calculations of energies and other observables (GFMC polishes VMC solutions down to the correct solution)

Barriers to getting ANCs from quantum Monte Carlo calculations

The VMC wave functions account very well for short-range correlations but generally get the long-range asymptotics wrong

Correcting the long-range problems without causing other problems is difficult

$C_{lj} = rR_{lj}(r)/W_{-\eta,l+\frac{1}{2}}(2kr)$ doesn't work because long-range shapes are generally wrong



Points are R_{lj} from VMC

Overlap is a Monte Carlo integration

Curve is $W_{-\eta,l+\frac{1}{2}}(2kr)/r$

Where do I match them?

Basis methods have the same problem

Integral relation for the ANC

There is a better way than explicit overlaps, ideally suited to QMC methods (appears in literature of 1960s, 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

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

which implies

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

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

Why is any of this useful?

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

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, $U_{\text{rel}} \to V_C$, so $U_{\text{rel}} - V_C \to 0$

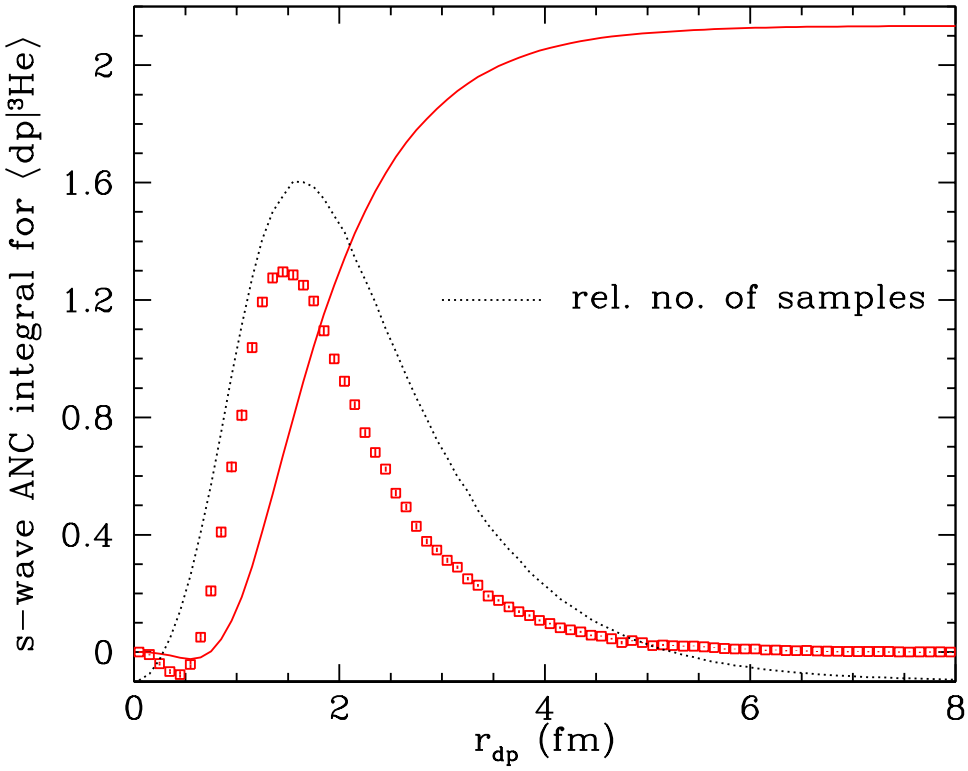
Integrand goes to zero at $\sim$ 7 fm with AV18+UIX

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

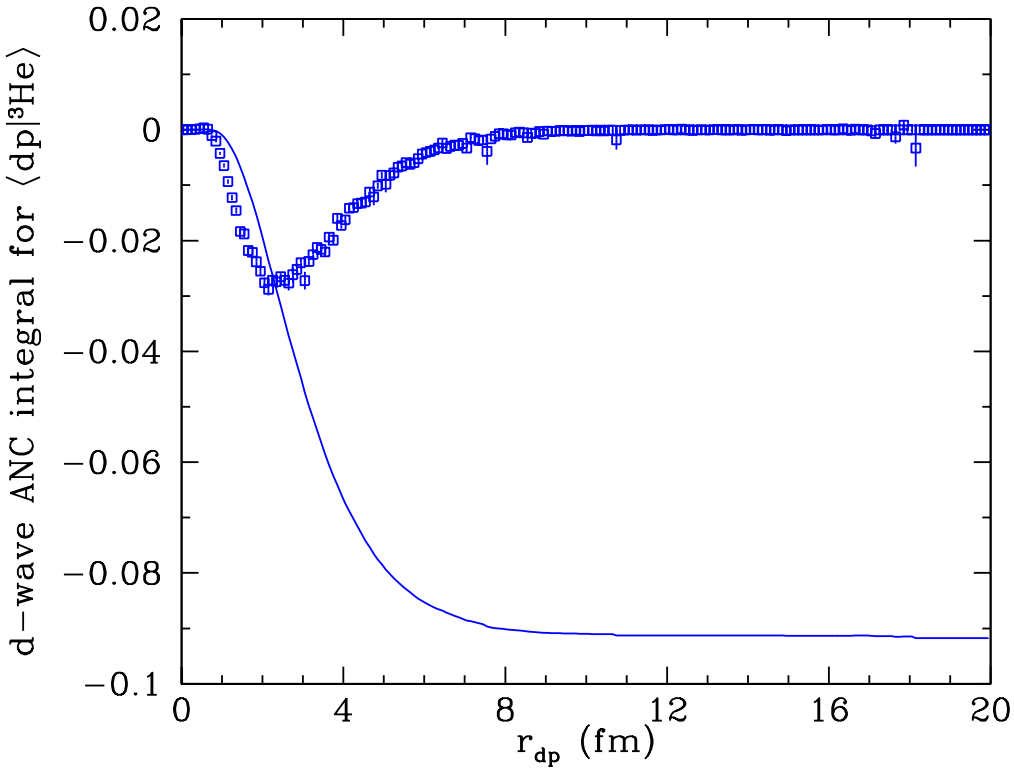
Closely related to Lippman-Schwinger equation (and to Pinkston-Satchler or Kawai-Yazaki)

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

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

Application to the VMC wave functions

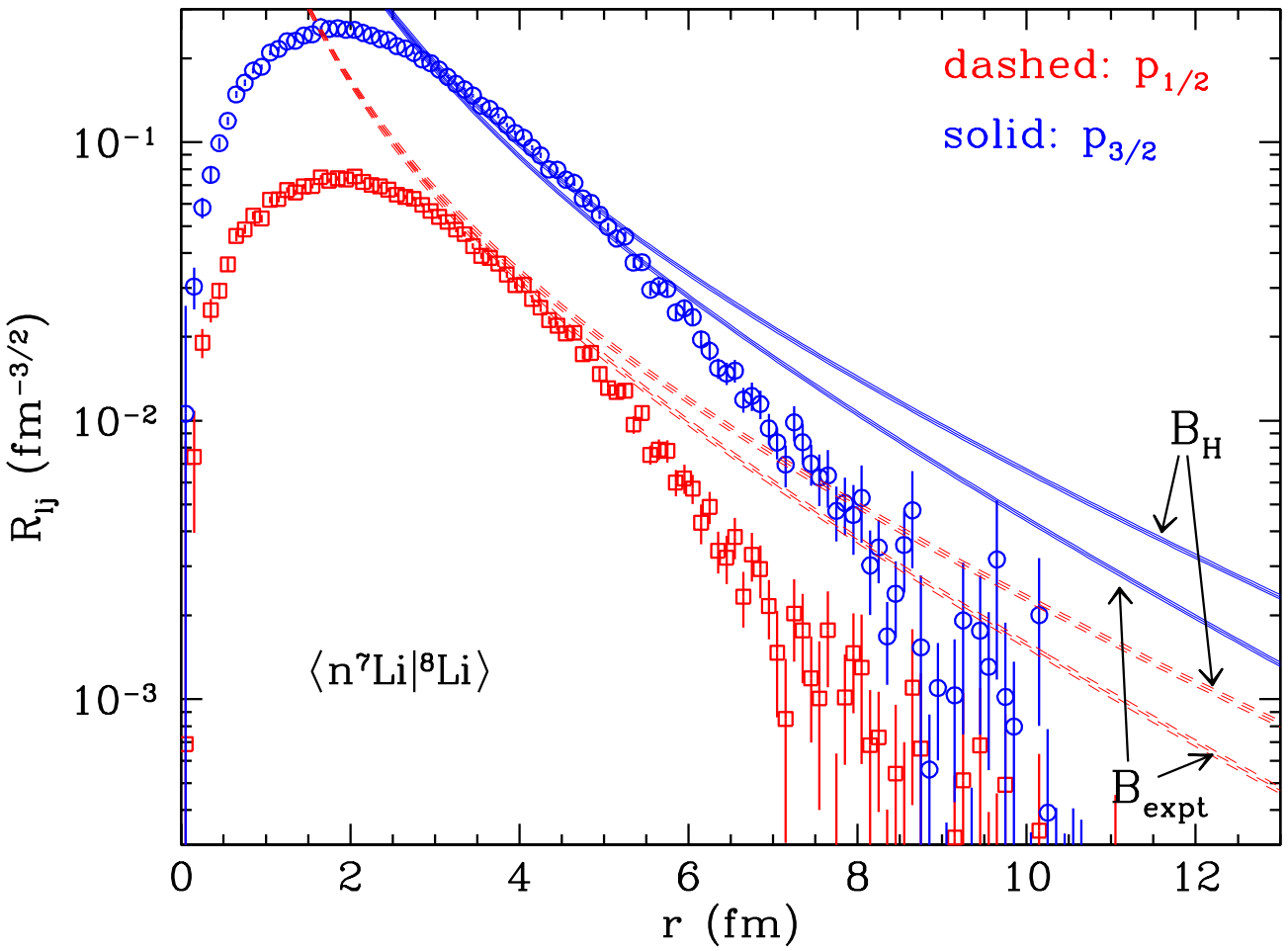
I've implemented the integral approach to the ANC within the VMC code, building on Wiringa's spectroscopic factor routines

I've applied the integral method to Wiringa's latest Argonne v_{18} + Urbana IX (AV18+UIX) wave functions for $A \leq 9$ in almost every combination of particle stable A- and $(A-1)$-body states

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

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



ANC (fm^{-1})	VMC: AV18+UIX binding	VMC: Lab binding	Experiment
$C^2_{p\,1/2}$	0.029(2)	0.048(3)	0.048(6)
$C^2_{p\,3/2}$	0.237(9)	0.382(14)	0.384(38)

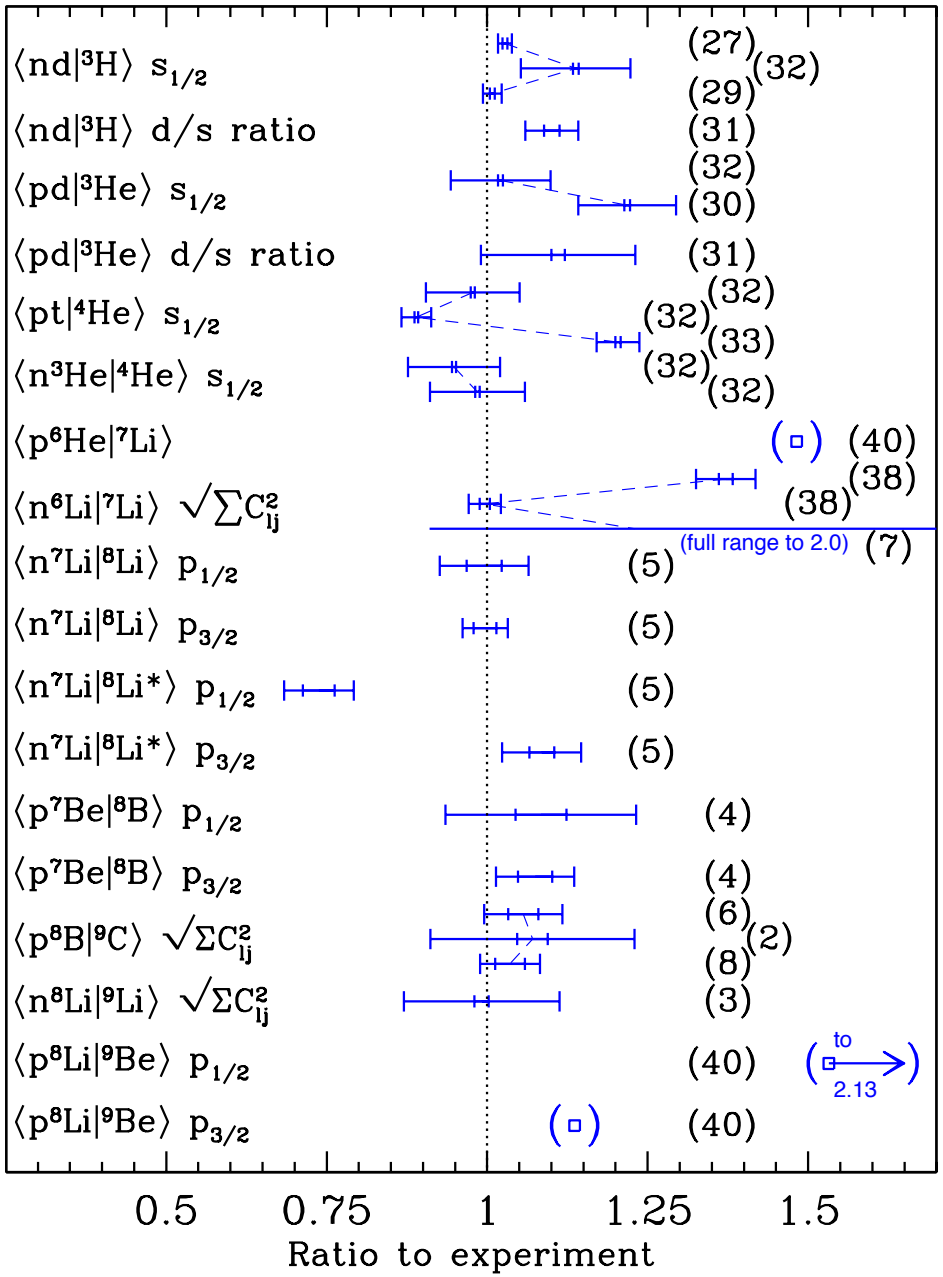
The results, $3 \leq A \leq 9$ one-nucleon removal

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

Readable results, where there are “experimental” data



Small error bars are VMC statistics

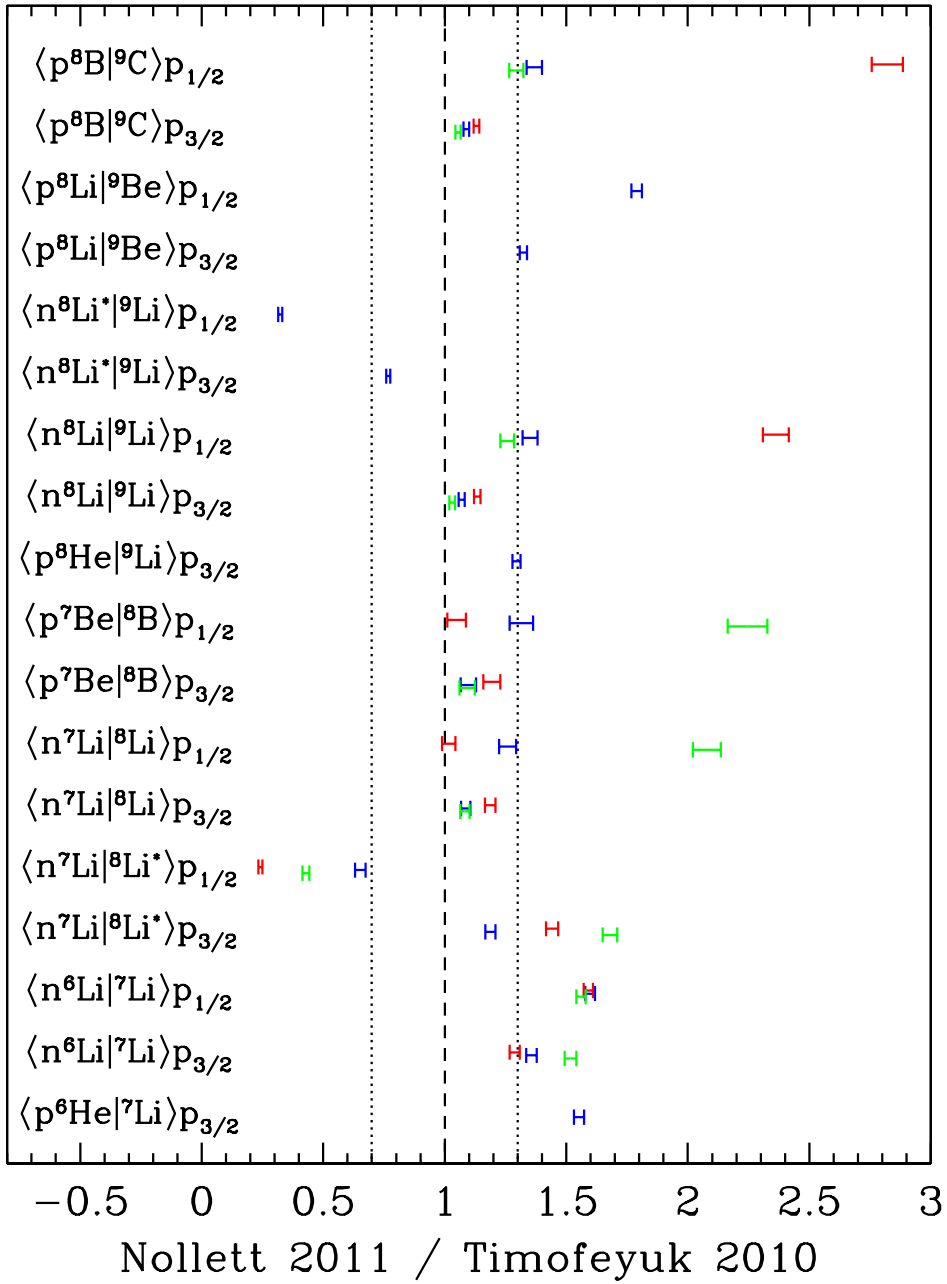
Large ones are “experimental”

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

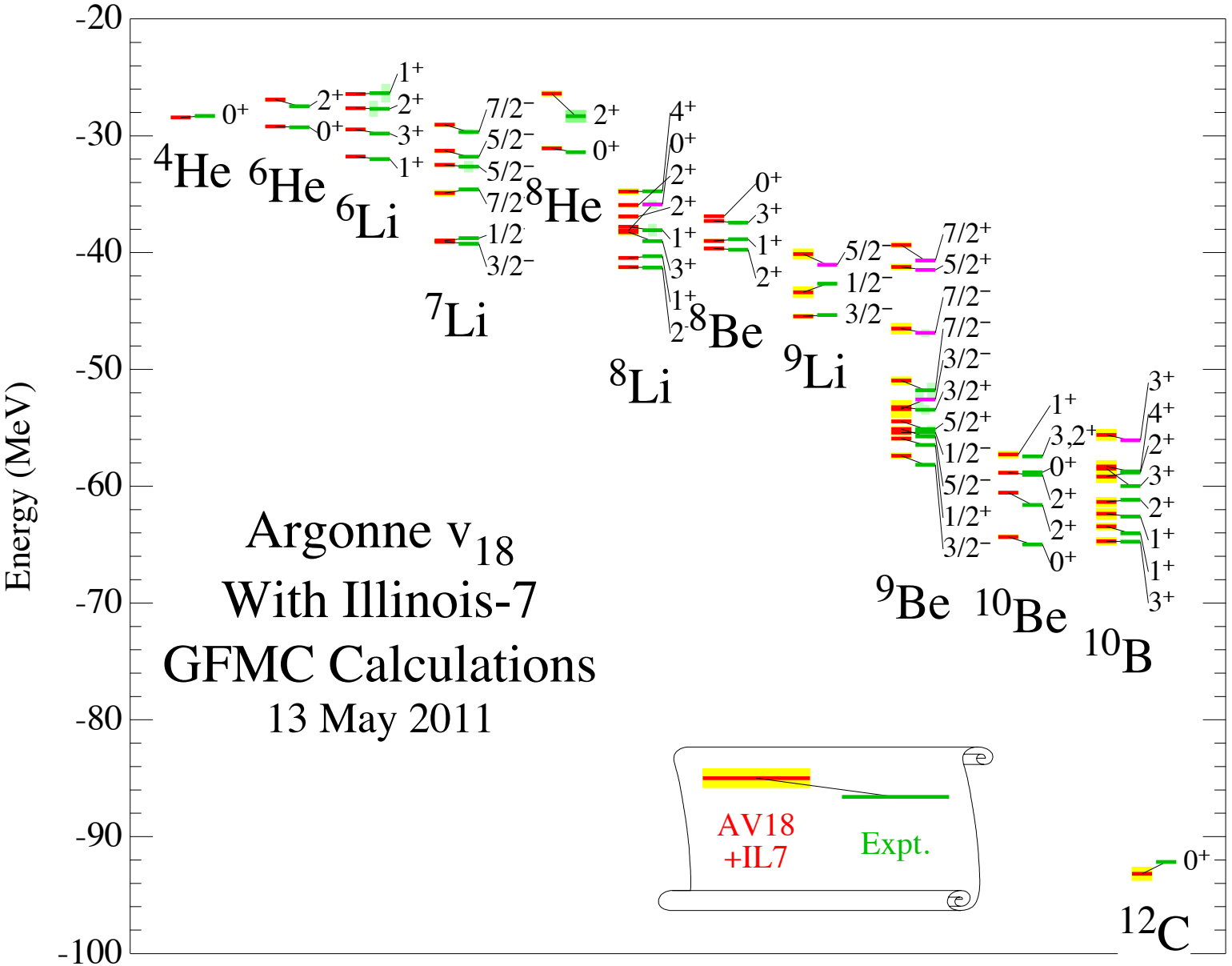
Possible extensions (bound states)

Cluster-cluster overlaps (e.g. $^7\mathrm{Be} \rightarrow \alpha\, ^3\mathrm{He}$) (needs reorganized code)

Application to GFMC solutions (and Illinois three-body force)

Computation of $R_{lj}(r)$ at all r – method as described is really the large-r limit of Pinkston-Satchler (or Kawai-Yazaki) overlaps

Many energies have been computed by QMC, but only two widths



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 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}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

An unbound wave function at large radius looks like

$$\psi(r \to \infty) \propto F_l(kr)\cos\delta + G_l(kr)\sin\delta$$

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

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

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

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

One could also consider Gamow's decaying complex-energy states (or Kapur-Peierls) and get the same answer

Widths as ANCs

The relation

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

for resonant states is mathematically almost the same as

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

for bound states

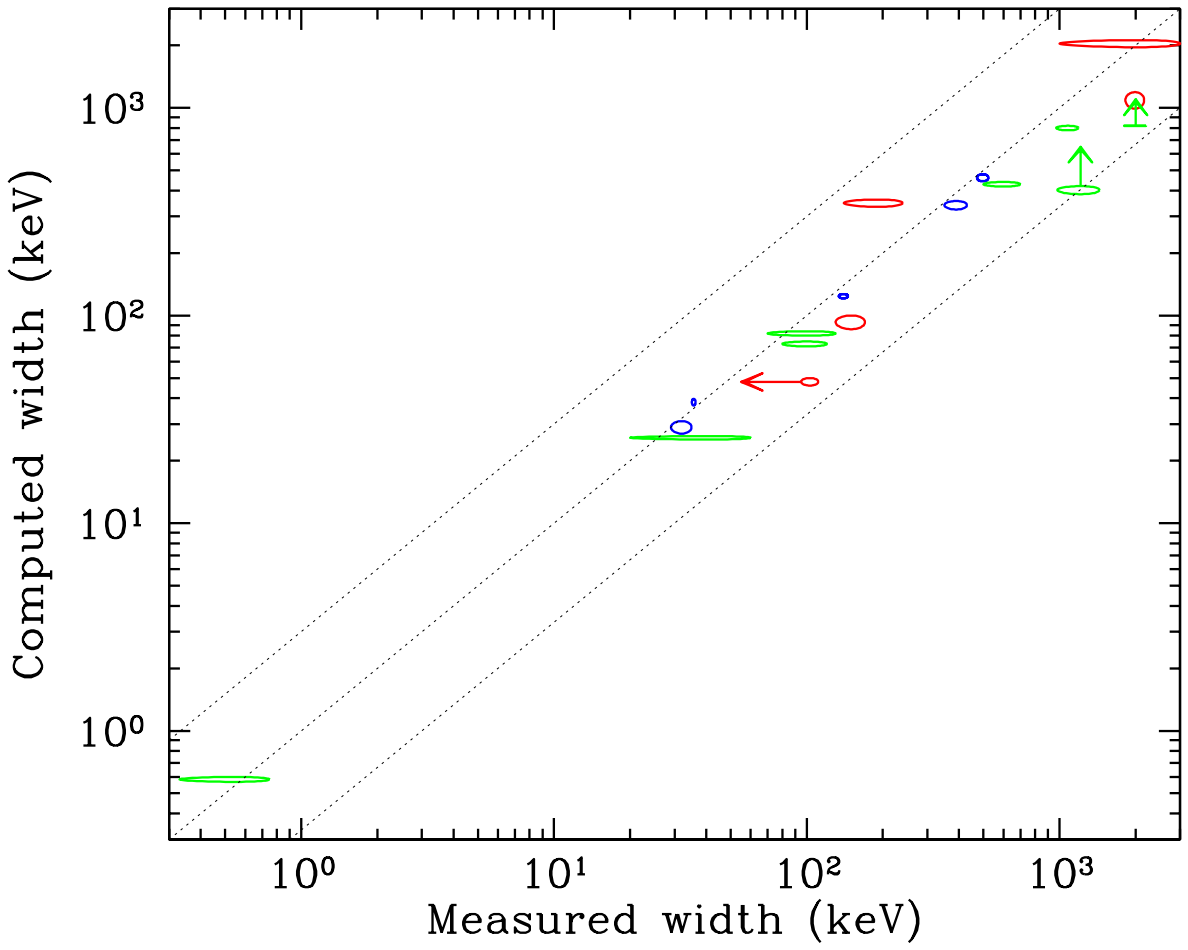
The integral method also applies to resonant states, except that now F_l appears in the integral instead of $M_{-\eta, l+\frac{1}{2}}$

This is used as a mathematical tool to get the asymptotics right in α and p decays (e.g. Esbensen & Davids (2000) deformed proton emitters, much Russian literature on α decay)

Testing out the integral relation for 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 width mainly/all in nucleon emission



A=7

A=8

A=9

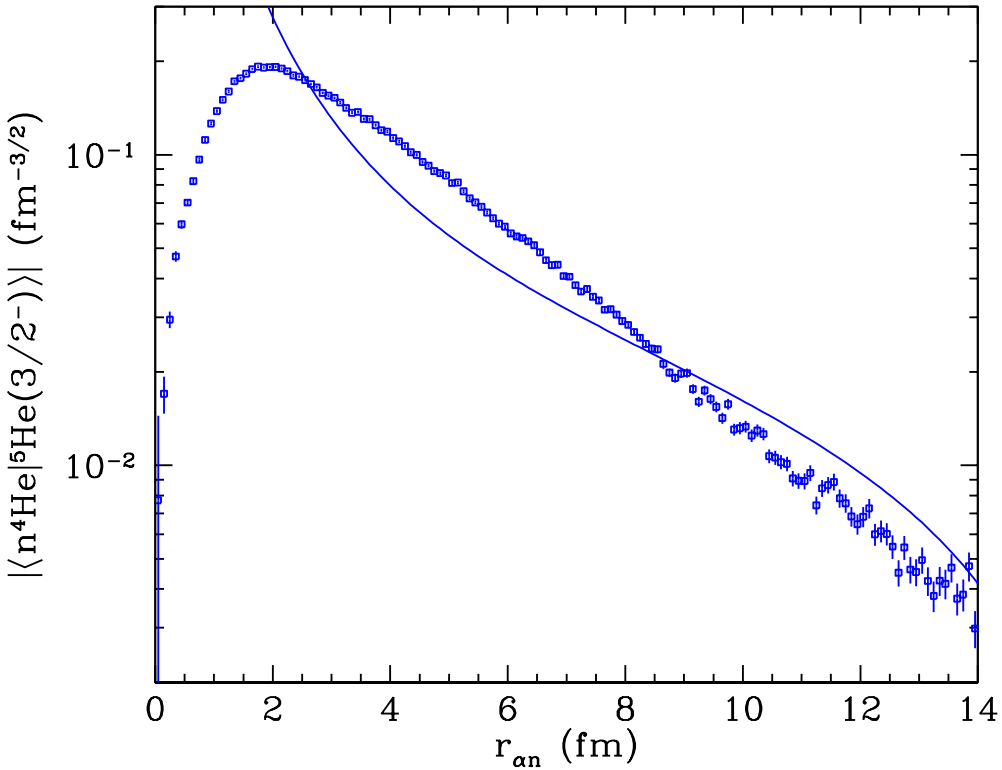
Arrows: uncomputed channels

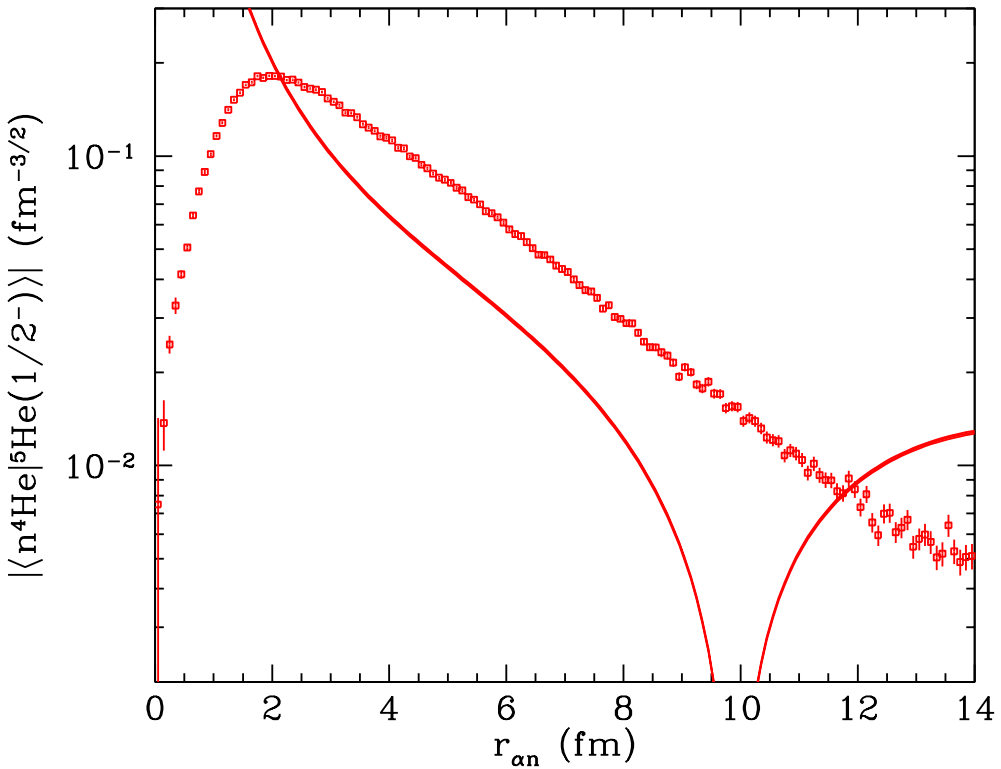
The good, the bad, the ugly

Lots of widths come out close to experiment

Widths not close to experiment generally have some unaccounted-for width (e.g. α or 3-body channel) or isospin mixing (^{8}Be 3^+ and 1^+ states), or are broad

Wiringa's pseudobound ^{5}He states yield wildly unreasonable widths, probably because they're very broad





Am I better off with the integral method than I was before?

I could have always made rough estimates of widths using computed S_{lj}

The method to beat is use of the Wigner (causality) limit of the width

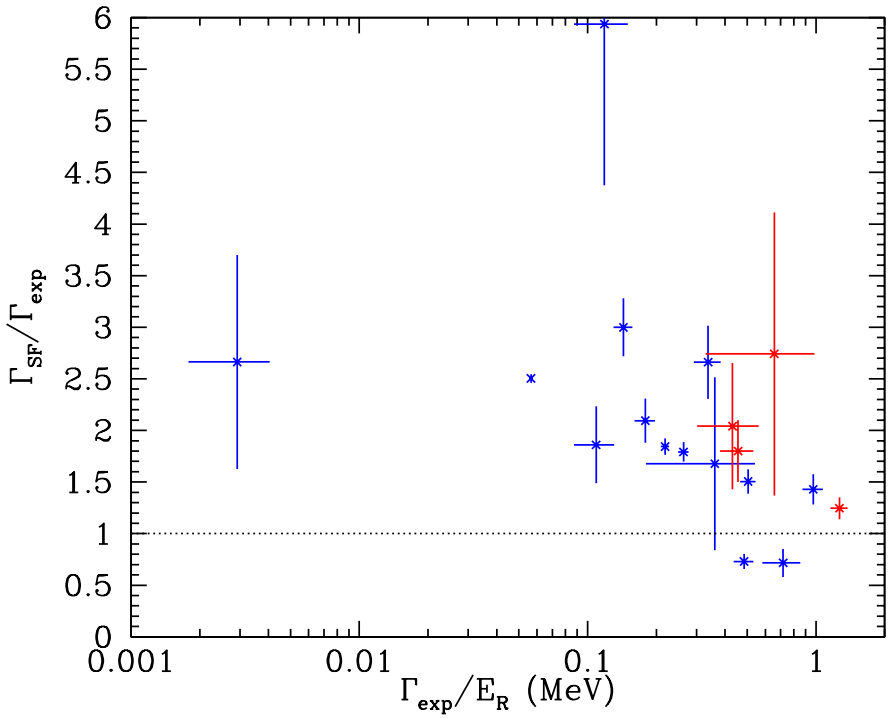
This is $\Gamma_W = 2\gamma_0^2 P_l(E)$ with $\gamma_0^2 = \frac{3\hbar^2}{2\mu r^2}$

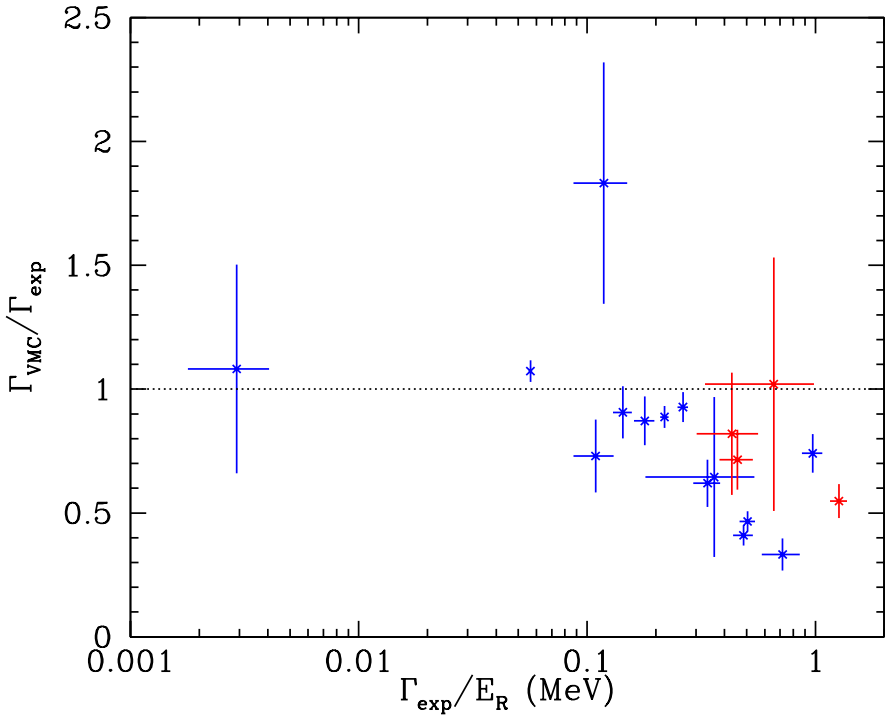
$P_l(E)$ is the barrier penetration factor of dispersion (R-matrix) theory

In terms of the dimensionless reduced width, the formal width is $\Gamma = \theta^2 \Gamma_W$

Since $\theta \lesssim 1$, it is tempting to identify it with spectroscopic factor, $S_{lj} \approx \theta^2$

Is the width integral better than using the Wigner limit and S_{lj}?





blue: consistent with 90° via P-S

red: not consistent

Note the different scales

For narrow states without open α channels, it's OK and apparently an improvement

Other cases still OK within a factor of ~ 2 (whether that's useful or not)

What next?

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

Tests against scattering calculations to see whether I can get the AV18+UIX widths this way

GFMC and IL7 (better match to experimental E_R)

Similar things are being done as pseudobound approaches to scattering $\delta(E)$ (Horiuchi et al., Kievsky et al., etc.) – maybe 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

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