

# ANCs, widths, and overlaps from integral relations

Kenneth Nollett  
Argonne National Laboratory

The Extreme Matter Physics of Nuclei:  
From Universal Properties to Neutron-Rich Extremes  
EMMI, GSI  
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Nollett & Wiringa, PRC 83, 041001(R) (2011), and in preparation  
(also other stuff)

## But what have you done for me lately?

*Ab initio* nuclear calculations have had great success over the past 15 years

Nuclear structure does indeed have quantitative roots in the vacuum NN interaction

Several features of light-nucleus energy spectra are reproduced:

- Overall scale of binding energy
- Orderings of  $J^\pi$  states (including  $^{10}\text{B}$  ground state, sensitive to NNN force)
- Spin-orbit splittings (also sensitive to NNN)

Quantum Monte Carlo achieved some of these things first

QMC dependence on  $A$  is steeper than Moore's Law, so it may not go beyond  $A = 12$  without some big change to algorithms

Many things remain to be done at  $A \leq 12$ : reactions, transitions, overlaps, etc.

## Quantum Monte Carlo, part I: Interactions

We work with the **Argonne  $v_{18}$**  nucleon-nucleon potential  
(18 operator terms, full EM, charge symmetry  
breaking,  $\chi^2_\nu = 1.09$ )



Three-nucleon interaction: Urbana IX fitted to  $^3\text{H}$  binding, saturation density  
Illinois-x fitted to 23 bound & narrow levels



VMC & GFMC as presently formulated need local interaction

## Quantum Monte Carlo, part II: Methods

We want to find nuclear energies and wave functions from the interaction

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$$

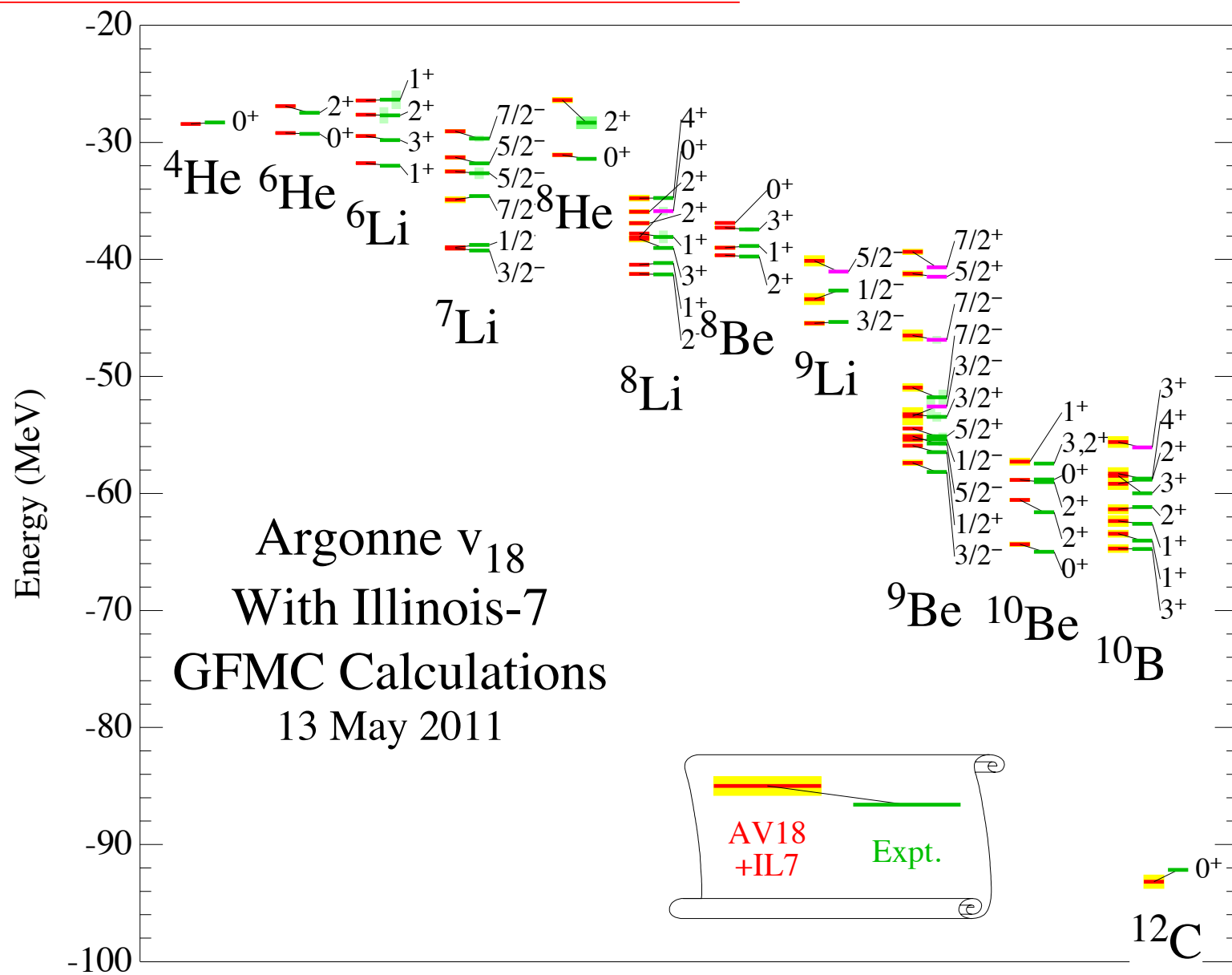
With one equation for each spin/isospin channel, this is some **270,000 coupled channels in 33 variables** for the case of  $^{12}\text{C}$

I use two methods as successive approximations:

- Variational Monte Carlo (VMC)
- Green's function Monte Carlo (GFMC)

Instead of a spatial basis, QMC methods operate on samples of the wave function at discrete points in the  $3A$ -dimensional configuration space

## A sampling of the quantum Monte Carlo results



## Quantum Monte Carlo results

The variational Monte Carlo (VMC) method give a first approximation, then Green's function Monte Carlo (GFMC) projects out the solution

Energies in 60 states up to  $A = 10$  are reproduced to better than 700 keV RMS (with four fitted parameters of the three-nucleon force)

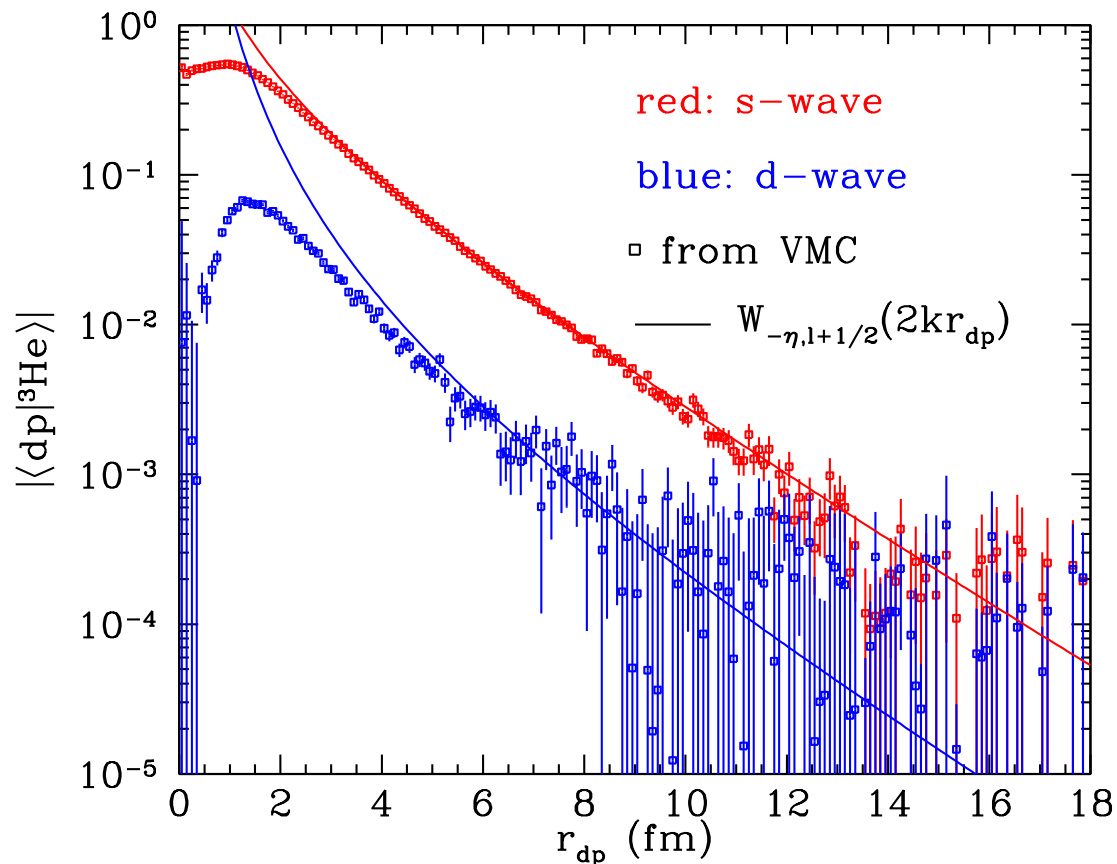
We have also successfully computed:

- RMS radii and quadrupole moments are computed, mostly with success
- $\beta$  and  $\gamma$  transition rates
- $\alpha + n$  scattering phase shifts
- pickup and stripping cross sections (via form factors & spectroscopic factors)
- $(e, e'p)$  cross sections

## Asymptotic normalization coefficient (ANC): definition

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

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



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

## Why 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 *ab initio* scattering/reaction calculations

“Indirect” approaches to ANCs might provide a path for improving asymptotic tails of QMC wave functions (quadrupole moments, etc.)



## 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  
→ ANCs  $\propto$  residues and can sometimes be extracted from analytically-continued scattering data (1970s)

Most ANC determinations (usually motivated by astrophysical capture) come 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

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

and particularly the spectroscopic factor

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

(though this is a questionable meeting point for theory and experiment; see recent papers by Mukhamedzhanov, Jennings, etc.)

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

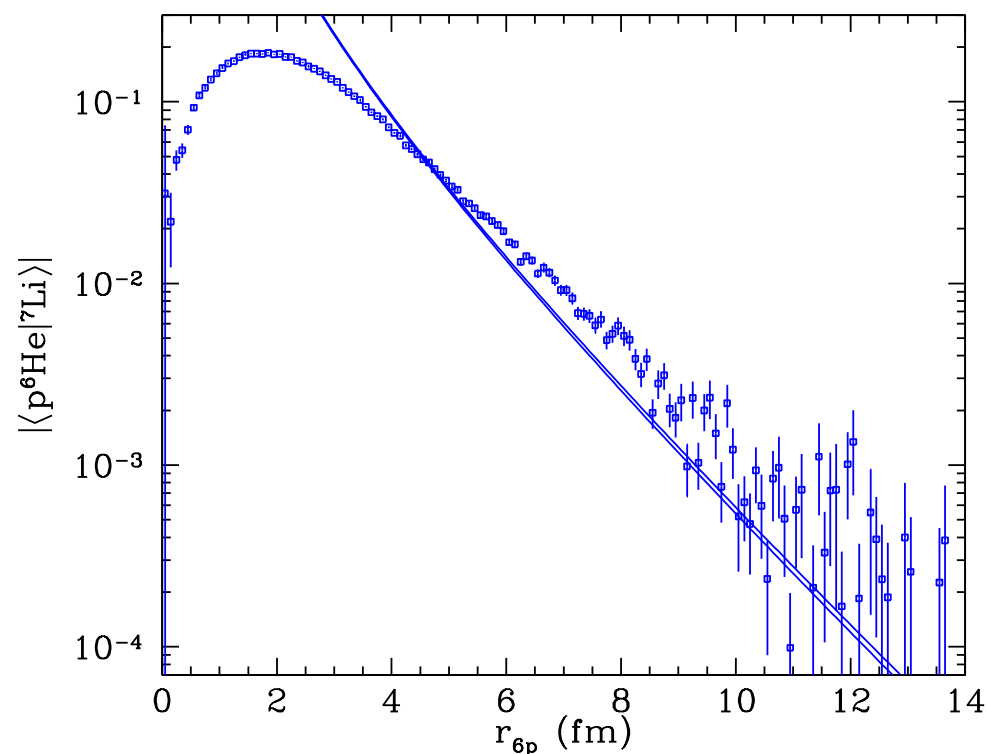
The VMC ansatz is very good and allows rather accurate calculations of energies and other observables (GFMC polishes VMC solutions down to the correct solution)

## 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 in a given clusterization channel without causing other problems is difficult (other channels get wrecked...)

$C_{lj} = rR_{lj}(r)/W_{-\eta,l+\frac{1}{2}}(2kr)$  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; 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

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

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

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

## 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  $U_{\text{rel}} - V_C \rightarrow 0$

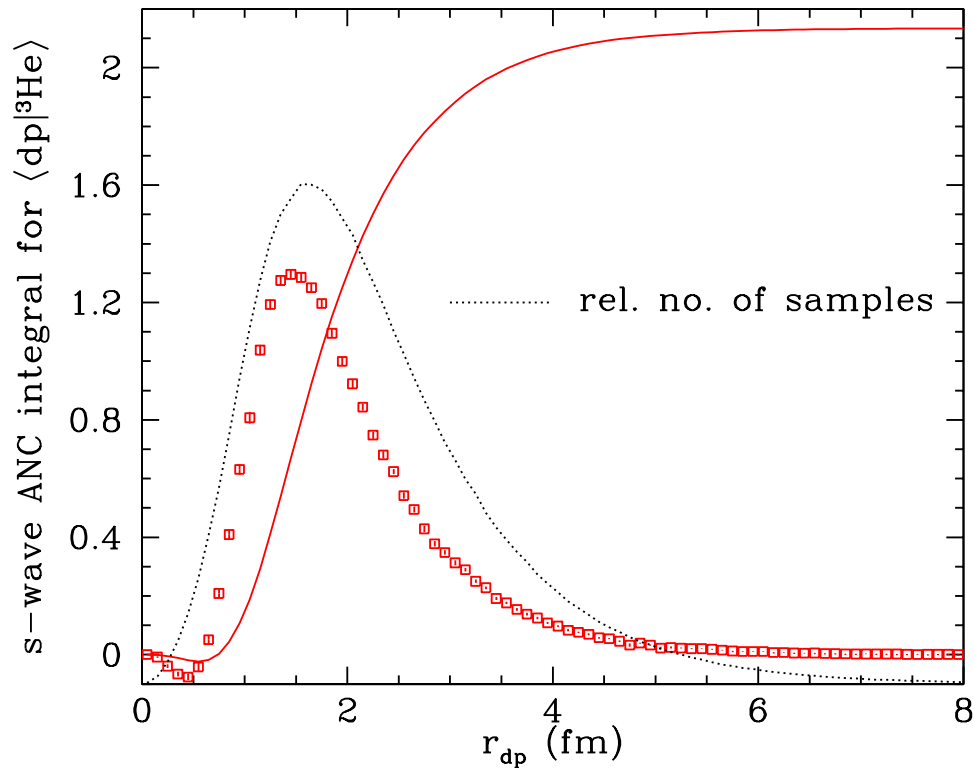
Integrand goes to zero at  $r_{cc} \sim 7$  fm with AV18+UIX

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

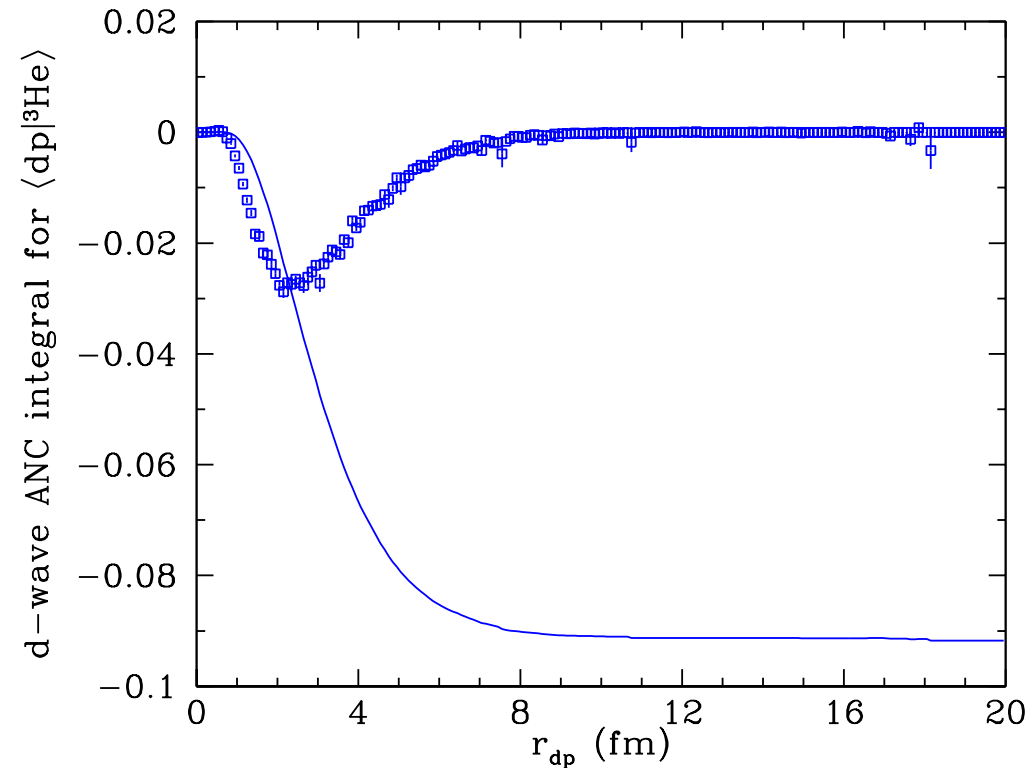
Closely related to Lippman-Schwinger equation (and to Pinkston-Satchler or Kawai-Yazaki overlaps); used by Mukhamedzhanov & Timofeyuk since  $\sim 1990$

## 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'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

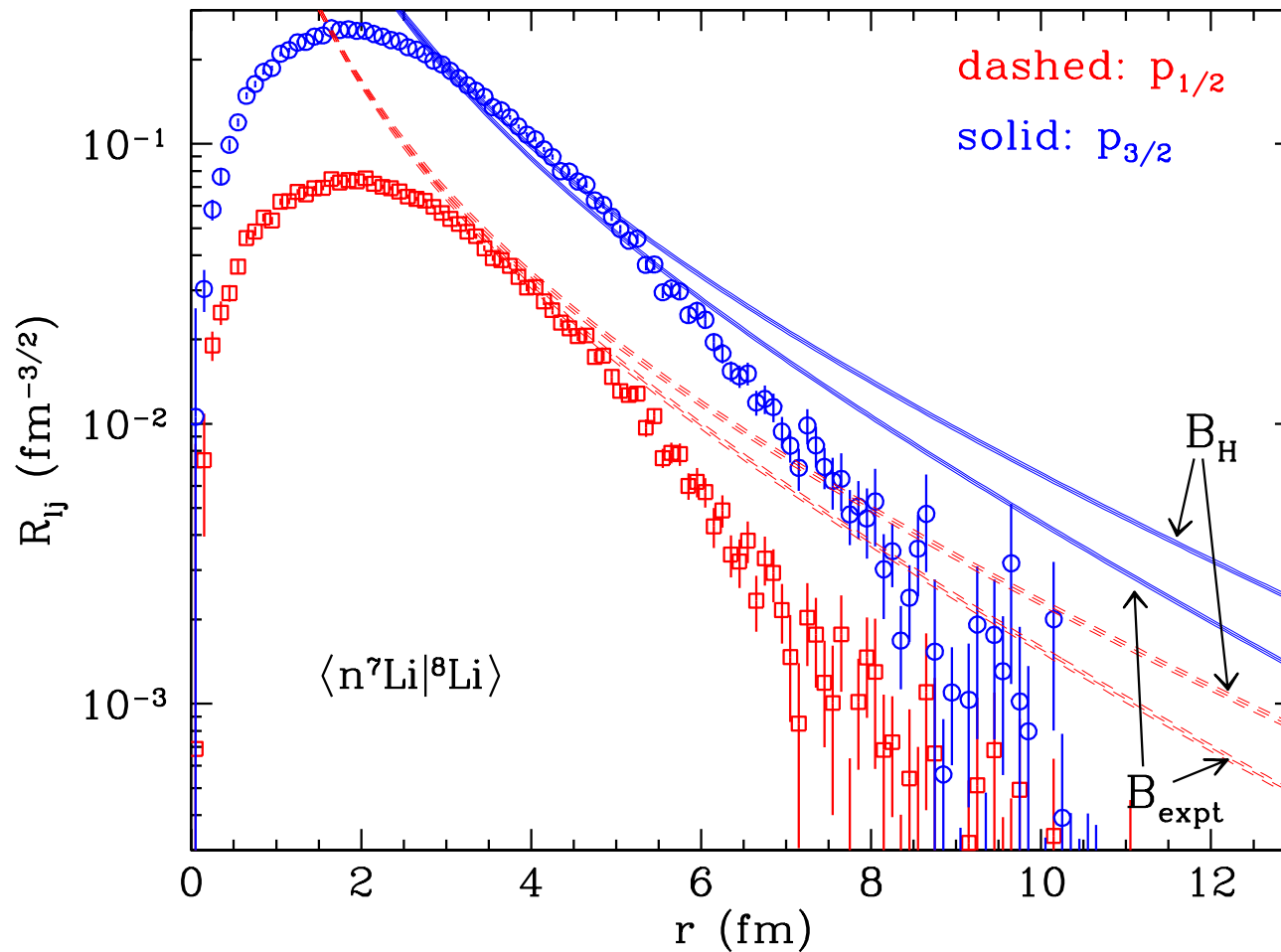
I have to choose a separation energy, either experimental or AV18+UIX, in evaluating each integral

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

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

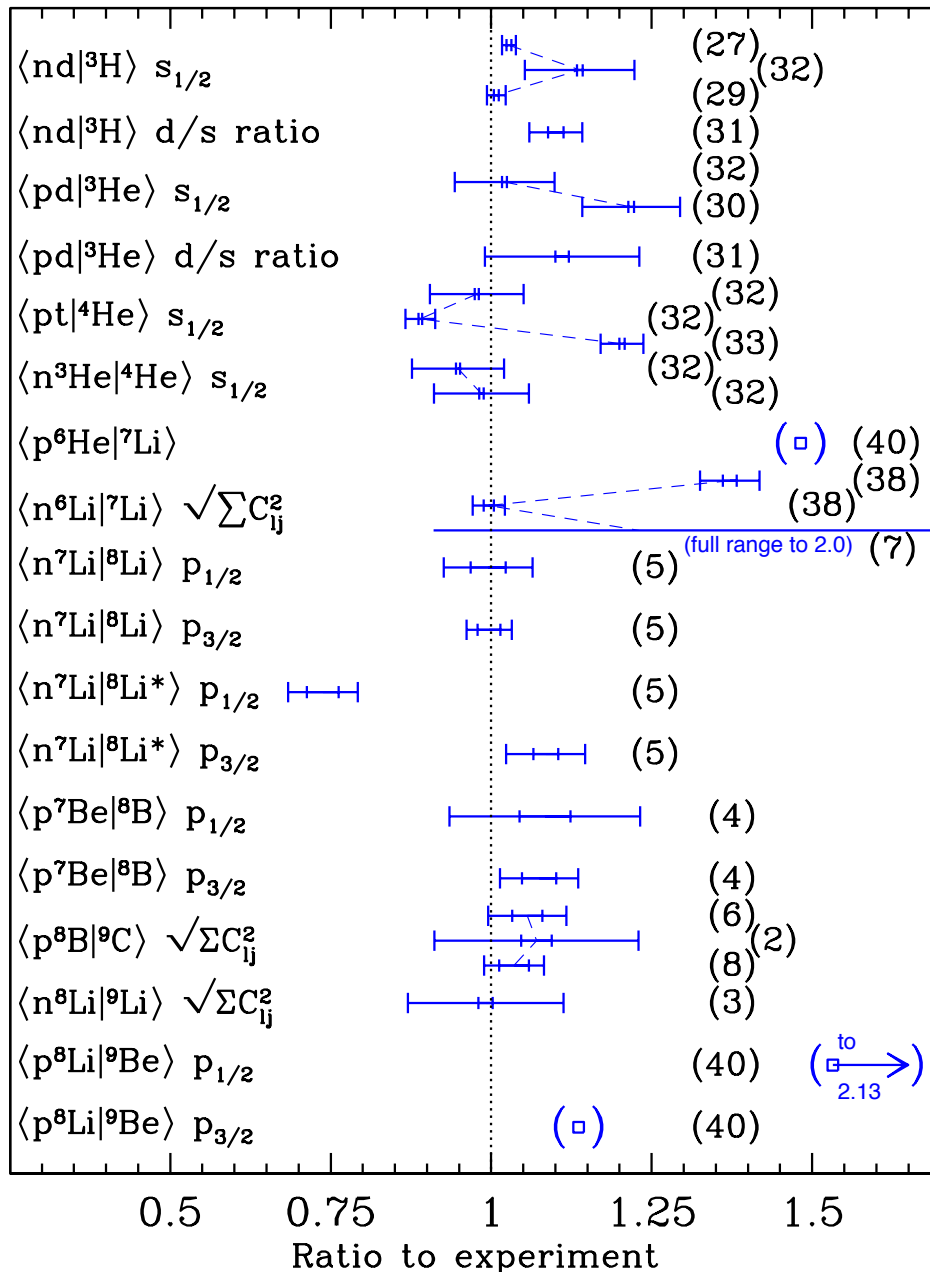


${}^8\text{Li} \rightarrow {}^7\text{Li} + n$  summarizes the whole project



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

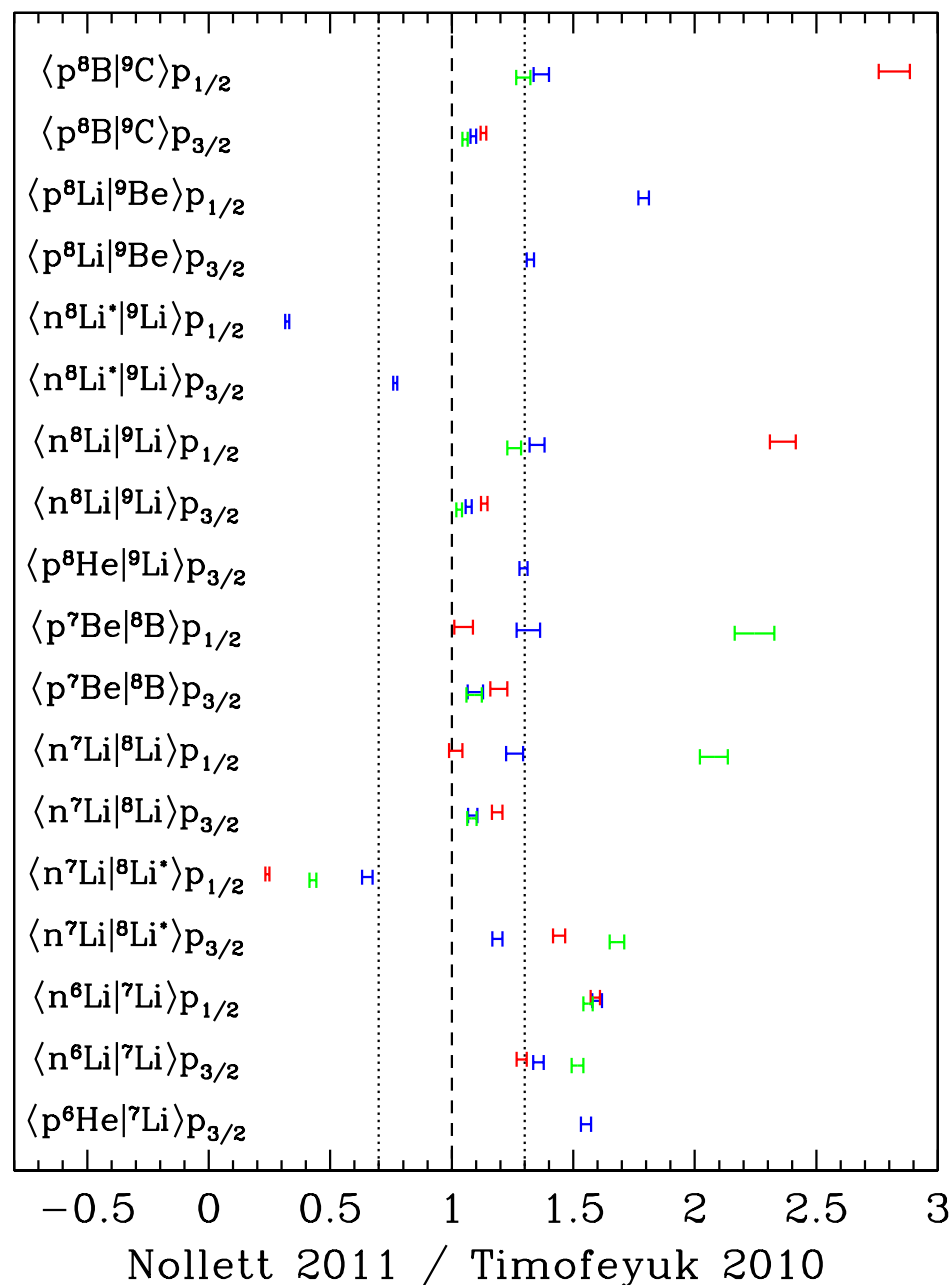
Large ones are “experimental”

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 *ab initio* 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 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

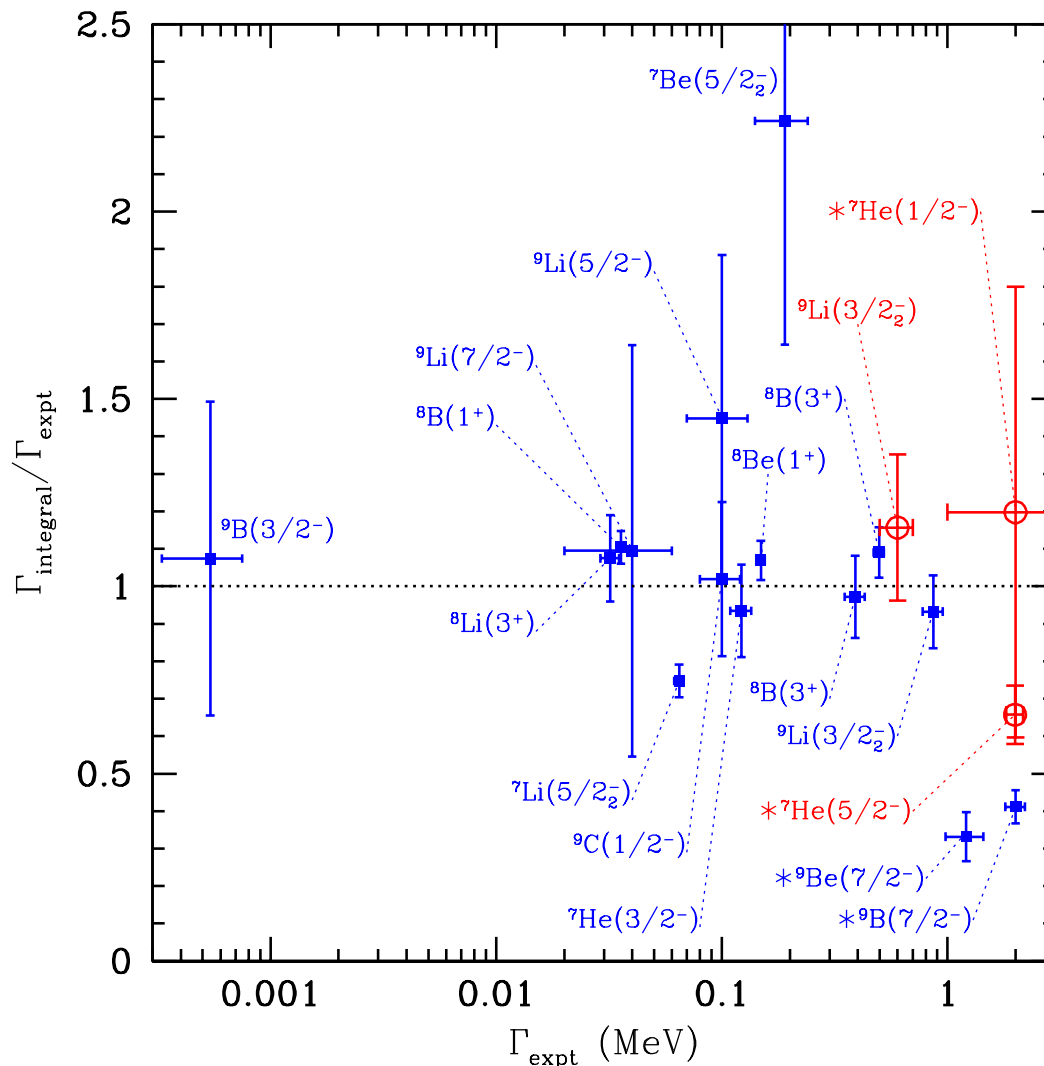
The integral method also applies to resonant states, except that now  $F_l$  appears in the integral instead of  $M_{-\eta, l+\frac{1}{2}}$

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 $\Gamma$

This has been a long time coming, paper in production now

State	Daughter	Experiment		From Exp energy $\Gamma_{VMC}$ (MeV)	From AV18+UIX energy		Matches 90°?	$\zeta$
		$E$ (MeV)	$\Gamma$ (MeV)		$E_{UIX}$ (MeV)	$\Gamma_{VMC}$ (MeV)		
$^6\text{He}(3/2^-)$	$^4\text{He}(0^+)$	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>		
$^7\text{He}(5/2^-)$	$^6\text{He}(2^+)$	1.57	1.99(17)	1.31(10) <sup>a</sup>	1.87	1.66(13) <sup>a</sup>	no	0.165
$^7\text{Li}(5/2^-)$	$^6\text{Li}(1^+)$	0.204	0.0646	0.0483(17) <sup>a</sup>	1.55	0.92(3) <sup>a</sup>	yes	0.055
$^7\text{Be}(5/2^-)$	$^6\text{Li}(1^+)$	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)		
$^9\text{Li}(3/2^-)$	$^8\text{Li}(2^+)$	1.316	—	0.522(13)	1.51	0.631(17)	no	0.014
$^9\text{Li}(3/2^-)$	$^8\text{Li}(1^+)$	0.340	—	0.172(4)	0.50	0.302(8)	yes	0.006
$^9\text{Li}(3/2^-)$	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

## Overlaps at all radii

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

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

$90^\circ$  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

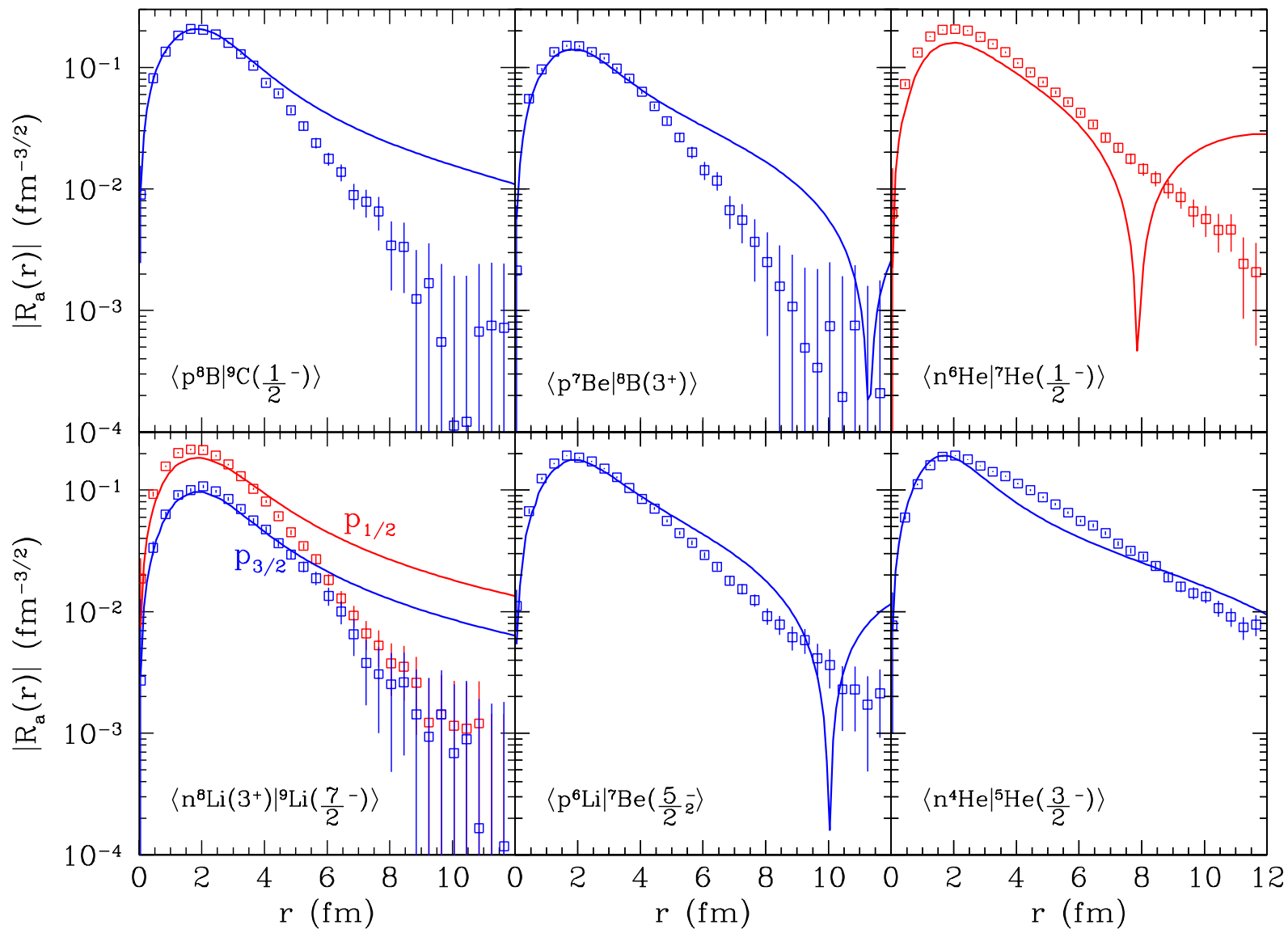
Cases that fail this test generally have small spectroscopic factors

## Overlaps at all radii

Good

Good

Bad

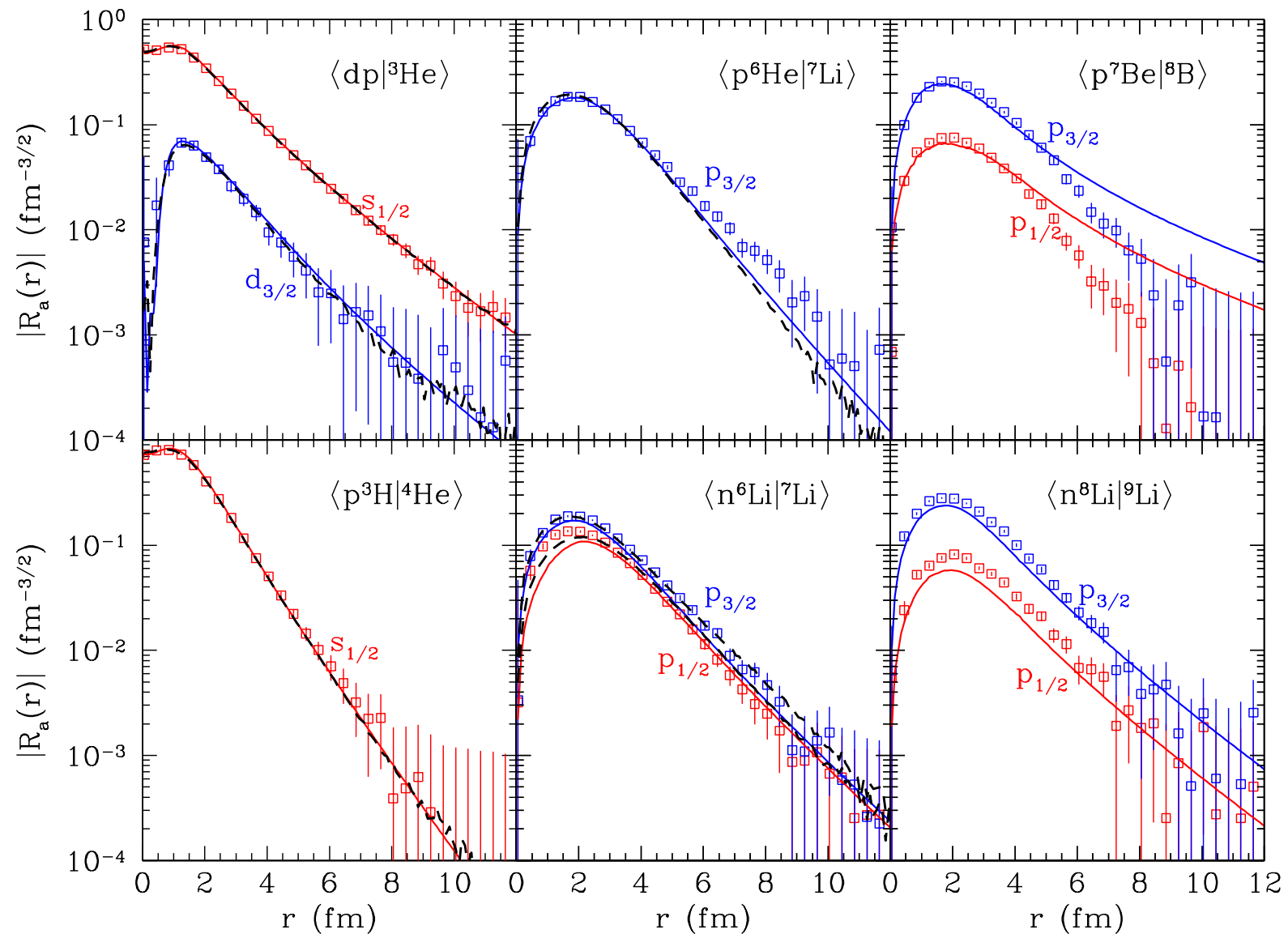


Points: Direct overlap

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



## Uses of overlaps

The overlap functions can help to make reaction theory consistent with structure theory (breakup,  $(d, p)$ ,  $(^3\text{He}, d)$ ...)

Several papers now use VMC overlaps (computed directly, not Pinkston-Satchler) as inputs via fitted Woods-Saxon wells:

$$(T + V_{\text{WS}})R_{lj} = ER_{lj}$$

with  $R_{lj}$  from VMC

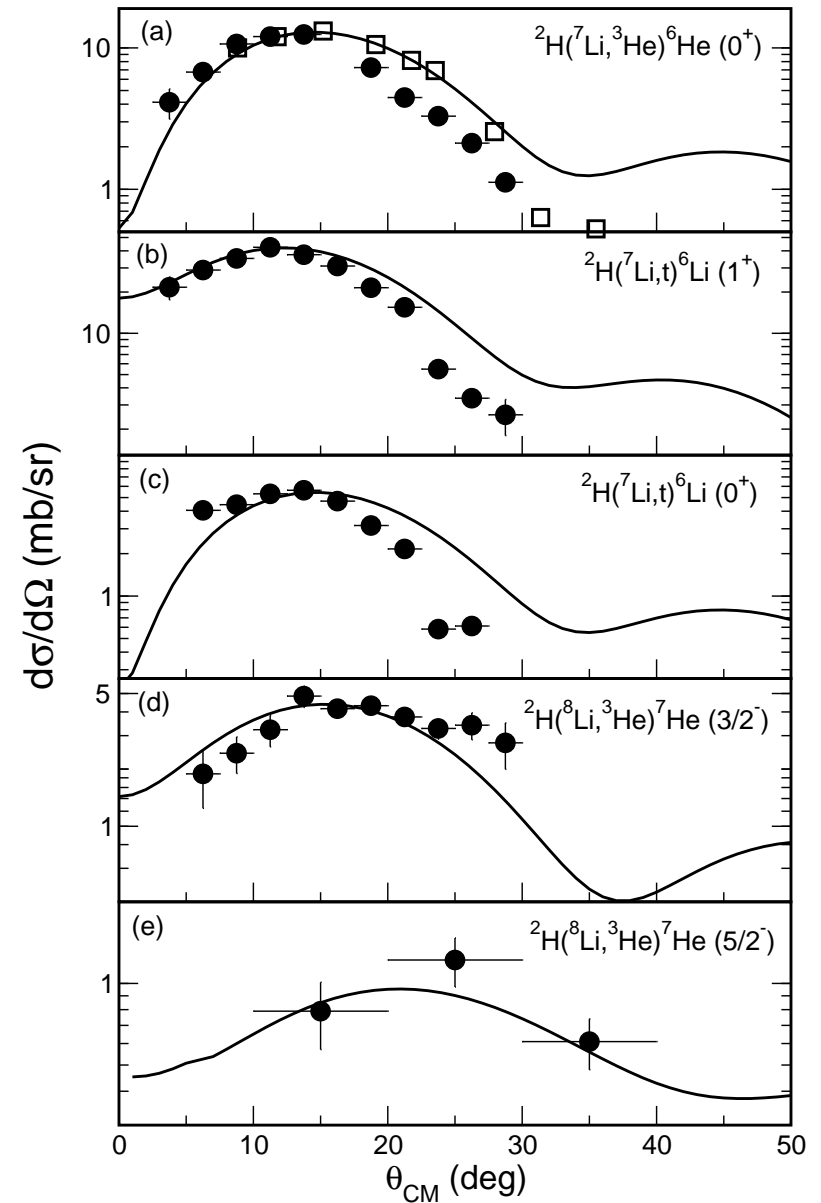
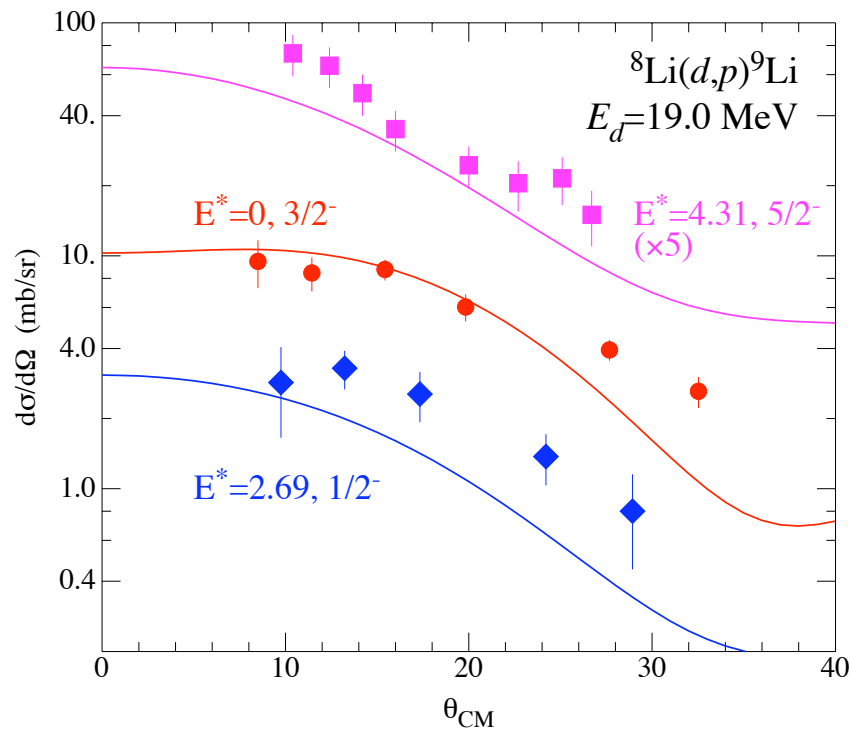
- Wuosmaa et al. PRC 72, 061301(R) (2005); PRL 94, 082502 (2005); PRC 78, 041302(R) (2008)
- Kanungo et al., PLB 660, 26 (2008)
- Grinyer et al. PRL 106, 162502 (2011)

With overlaps as input & no further fudging, experiment & VMC results agree (same spectroscopic factor – even for  $^7\text{Li}$ , *pace* ubiquitous graphs)

## Some examples

DWBA with  $\langle A-1|A \rangle$  vertices from VMC overlaps

There's still an optical potential, e.g. for  ${}^8\text{Li}+d$



## Integral method vs. factorized widths from spectroscopic factors

I could have always made rough estimates of widths using a factorization  $S_{lj}\Gamma_{\text{s.p.}}$ ,  
with  $S_{lj}$  from QMC

Wigner (causality) limit is easy to use for  $\Gamma_{\text{s.p.}}$  but not much good

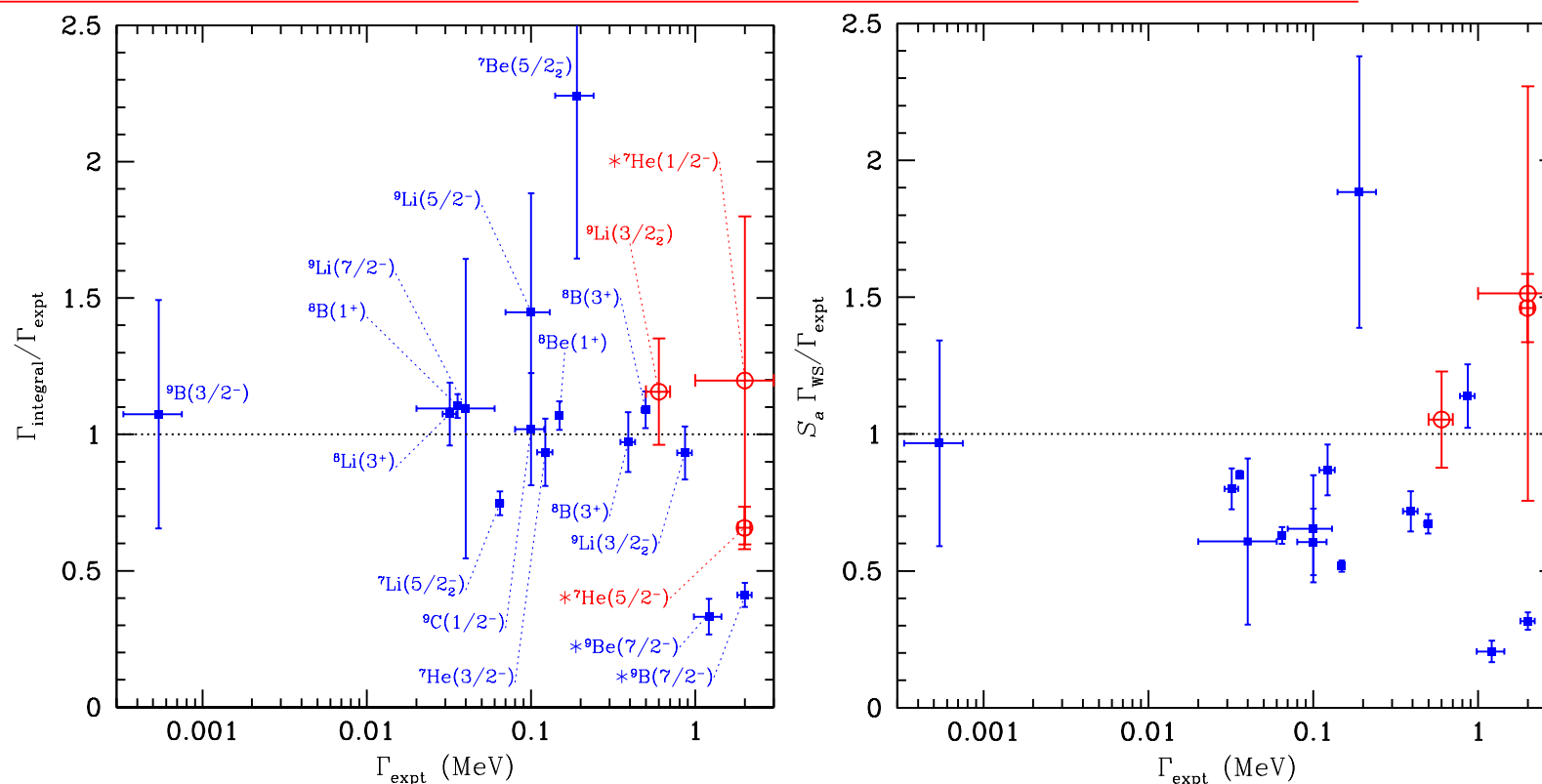
Shell-model studies often use “single-particle” widths computed from Woods-Saxon well

“Standard” geometric parameters are used & depth is set to match resonance energy, obtaining  $\Gamma_{\text{WS}}$

This width is multiplied by the spectroscopic factor:  $S_{lj}\Gamma_{\text{WS}}$

Geometric parameters should then be varied within “reasonable” bounds to check sensitivity

# Is the width integral better than the Woods-Saxon width times $S_{lj}$ ?



blue: consistent with  $90^\circ$  via P-S

red: not consistent

For narrow states without open  $\alpha$  channels, it's good and apparently an improvement

Mean of vertical axis, states where all channels counted & VMC wave function

“looks resonant:”  $1.06 \pm 0.07$  integral,  $0.75 \pm 0.15$  Woods-Saxon

( $\chi^2_\nu = 1.5$  vs. 34)



## Widths and state identification: ${}^7\text{He}$ & ${}^9\text{Li}$

New theoretical information should be useful for  $J^\pi$  identification of states

The  ${}^7\text{He}$  ground state ( $\frac{3}{2}^-$ ) is not too bad:  $\Gamma = 114(4) \text{ keV}$  vs.  $\Gamma = 125_{-15}^{+40}$  measured

Neither  ${}^7\text{He}(\frac{1}{2}^-)$  nor  ${}^7\text{He}(\frac{5}{2}^-)$  overlaps look like  $90^\circ$  phase shift (both are broad);  $\frac{1}{2}^-$  width isn't bad

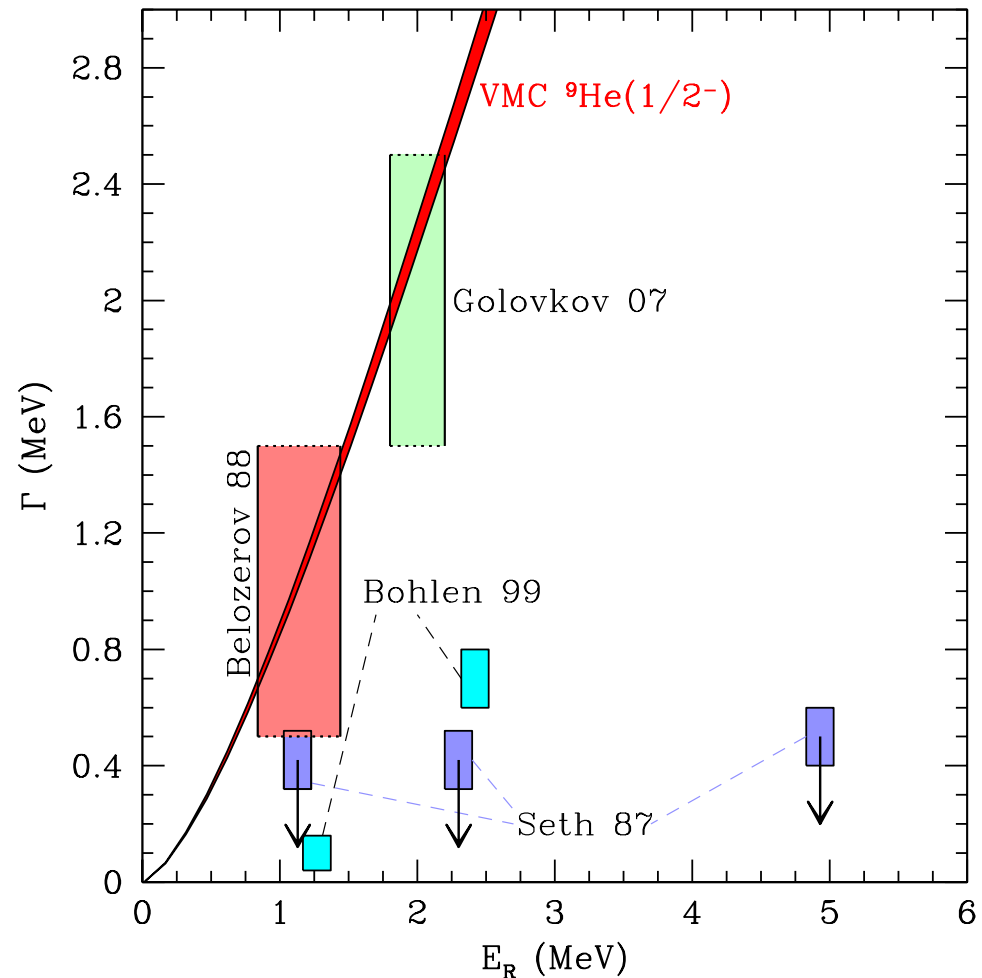
Computed  ${}^9\text{Li}$  widths support  $J^\pi$  assignments of Wuosmaa *et al.* 2005:  
 $3/2^-$ ,  $1/2^-$ ,  $5/2^-$ ,  $3/2^-$ ,  $7/2^-$

## Widths and state identification: $^9\text{He}$

Broad  $\frac{1}{2}^-$  matches width claimed at Dubna (but not elsewhere)

I find  $< 5$  keV width for  $\frac{3}{2}^-$ , but direct overlap is inconsistent with  $90^\circ$

Did not consider unbound decay products (so no decays through  $^8\text{He}(2^+)$ )



There should be even-parity intruders, but those VMC aren't well developed, and  $^8\text{He}(2^+)$  should be important

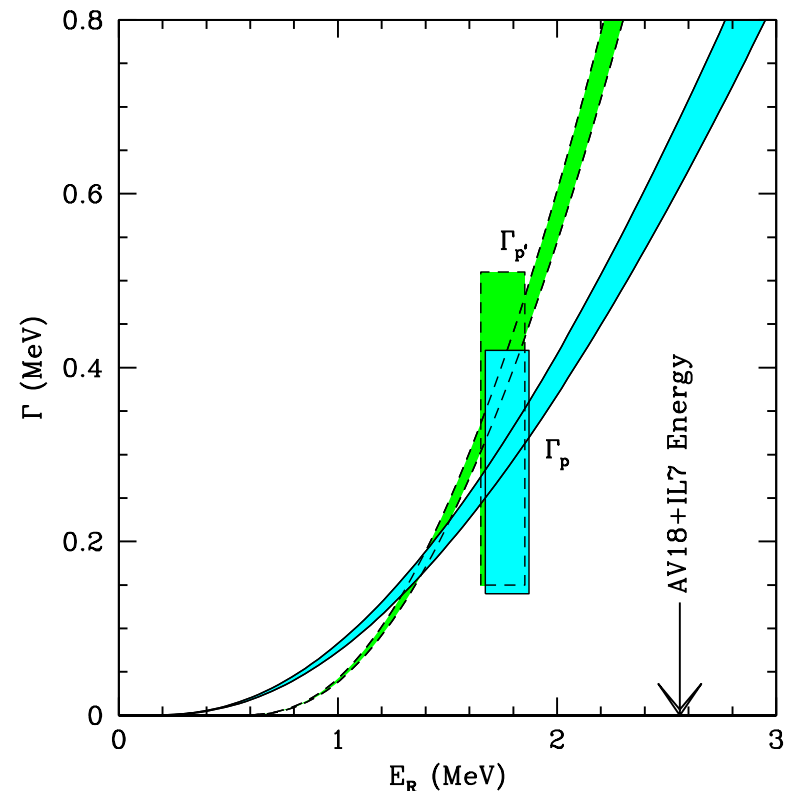
## Widths and state identification: $^8\text{B}$

Mitchell *et al.* 2010 claim new broad  $0^+$  &  $2^+$  states in  $^8\text{B}$  (at low significance)

$0^+$  width calculations look unreliable –  
90° test failed

I can assume a range of  $E$  in the width  
and see what  $\Gamma$  corresponds

Widths to  $^7\text{Be}$  &  $^7\text{Be}^*$  computed  
separately



VMC  $2^+$  states are compatible with 90°, but I don't reproduce Mitchell widths  
of  $^8\text{B}(2_2^+)$  state

## What next?

$\alpha$  (and other cluster) widths & overlaps 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 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

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