## QMC Calculations of Light Nuclei – More Than Just Energies –

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WORK WITH

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WORK NOT POSSIBLE WITHOUT EXTENSIVE COMPUTER RESOURCES Argonne Laboratory Computing Resource Center (Fusion) Argonne Math. & Comp. Science Division (SiCortex) Argonne Leadership Computing Facility (BlueGene/P)



**Physics Division** 

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#### GOALS

Understand nuclei at the level of elementary interactions between individual nucleons, including

- Binding energies, excitation spectra, relative stability, widths
- Densities, electroweak transitions, cluster-cluster overlaps & spectroscopic factors
- Low-energy NA & AA' scattering, astrophysical reactions, asymptotic normalizations

#### REQUIREMENTS

- Two-nucleon potentials that accurately describe elastic NN scattering data
- Consistent three-nucleon potentials and electroweak current operators
- Precise methods for solving the many-nucleon Schrödinger equation

#### RESULTS

- Quantum Monte Carlo methods can evaluate realistic Hamiltonians accurate to  $\sim 1-2\%$
- About 100 states calculated for  $A \le 12$  nuclei in good agreement with experiment
- ${}^{5}\text{He} = n\alpha$  scattering and low-energy electroweak astrophysical reactions
- Applications to elastic & ineleastic  $e, \pi$  scattering, (e, e'p), (d, p) reactions, etc.



$$H = \sum_{i} K_i + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk}$$

 $K_i$ : Non-relativistic kinetic energy,  $m_n$ - $m_p$  effects included

Argonne v<sub>18</sub>:  $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij})O_{ij}^p$ 

- 18 spin, tensor, spin-orbit, isospin, etc., operators
- full EM and strong CD and CSB terms included
- predominantly local operator structure
- fits Nijmegen PWA93 data with  $\chi^2$ /d.o.f.=1.1

Wiringa, Stoks, & Schiavilla, PRC 51, (1995)

Urbana & Illinois:  $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^{R}$ 

- Urbana has standard  $2\pi P$ -wave + short-range repulsion for matter saturation
- Illinois adds  $2\pi$  S-wave +  $3\pi$  rings to provide extra T=3/2 interaction
- Illinois-7 has four parameters fit to 23 levels in  $A \leq 10$  nuclei

Pieper, Pandharipande, Wiringa, & Carlson, PRC **64**, 014001 (2001) Pieper, AIP CP **1011**, 143 (2008)





### QUANTUM MONTE CARLO

#### Variational Monte Carlo (VMC): construct $\Psi_V$ that

- Are fully antisymmetric and translationally invariant
- Have cluster structure and correct asymptotic form
- Contain non-commuting 2- & 3-body operator correlations from  $v_{ij} \& V_{ijk}$
- Are orthogonal for multiple  $J^{\pi}$  states
- Minimize  $E_V = \langle \Psi_V | H | \Psi_V \rangle \geq E$

These are  $\sim 2^A \begin{pmatrix} A \\ Z \end{pmatrix}$  component spin-isospin vectors in 3A dimensions

#### Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H E_0)\tau]\Psi_V = \sum_n \exp[-(E_n E_0)\tau]a_n\Psi_n \Rightarrow \Psi_0$  at large  $\tau$
- Propagation done stochastically in small time slices  $\Delta\tau$
- Exact  $\langle H \rangle$  for local potentials; mixed estimates  $\langle \Psi_V | O | \Psi(\tau) \rangle$  for other operators
- Constrained-path propagation controls fermion sign problem for  $A \ge 5$
- Multiple excited states for same  $J^{\pi}$  stay orthogonal

#### Many tests demonstrate 1–2% accuracy for realistic $\langle H \rangle$

Pudliner, Pandharipande, Carlson, Pieper, & Wiringa, PRC 56, 1720 (1997)
Wiringa, Pieper, Carlson, & Pandharipande, PRC 62, 014001 (2000)
Pieper, Varga, & Wiringa, PRC 66, 044310 (2002)
Pieper, Wiringa, & Carlson, PRC 70, 054325 (2004)





### APPLICATIONS TO LIGHT-ION REACTIONS

The availability of radioactive-ion beams has renewed interest in reactions like (d,p) in inverse kinematics

We have helped analyze a number of RIB experiments such as  $d({}^{8}\text{Li},p){}^{9}\text{Li}$  (ATLAS) &  $d({}^{9}\text{Li},t){}^{8}\text{Li}$  (TRIUMF)

- PTOLEMY DWBA calculations for transfer
- (d,p) vertex from AV18
- (d,t), (<sup>8</sup>Li,<sup>9</sup>Li), etc. vertices computed as *A*-body overlaps using VMC  $\langle \Psi_V(A-1) | a | \Psi_V(A) \rangle$
- Norm is spectroscopic factor
- Absolute prediction for  $d\sigma/d\Omega$
- Good predictions of *n*-knockout from <sup>10</sup>Be and <sup>10</sup>C (NSCL)

Macfarlane & Pieper, PTOLEMY, ANL-76-11, Rev. 1 (1978) Wuosmaa *et al.*, PRL **94**, 082502 (2005) + ... Kanungo *et al.*, PLB **660**, 26 (2008) Grinyer *et al.*, PRL **106**, 162502 (2011)



### **ONE-NUCLEON OVERLAPS IN VMC/GFMC**

For antisymmetric and translationally invariant parent  $\Psi_A(\alpha)$  and daughter  $\Psi_{A-1}(\gamma)$  wave functions, with  $\alpha \equiv [J_A^{\pi}, T_A, T_{z_A}], \gamma \equiv [J_{A-1}^{\pi}, T_{A-1}, T_{z_{A-1}}]$ , and single-nucleon quantum numbers  $\nu \equiv [l, s, j, t, t_z]$ , the translationally invariant overlap function is:

$$R(\alpha,\gamma,\nu;r) = \sqrt{A} \left\langle \left[ \Psi_{A-1}(\gamma) \otimes \mathcal{Y}(\nu)(\hat{r}') \right]_{J_A,T_A} \left| \frac{\delta(r-r')}{r^2} \right| \Psi_A(\alpha) \right\rangle$$

where  $\mathcal{Y}(\nu)(\hat{r}') = [Y_l(\hat{r}') \otimes \chi_s]_j \chi_t$  and  $|\Psi_{A-1}(\gamma)|^2 = 1, |\Psi_A(\alpha)|^2 = 1.$ 

The corresponding spectroscopic factor is the norm of the overlap:

$$S(lpha,\gamma,
u)=\int |R(lpha,\gamma,
u;r)|^2 r^2 dr$$

Overlap functions R satisfy a one-body Schrödinger equation with appropriate source terms. Asymptotically, at  $r \to \infty$ , these source terms contain core-valence Coulomb interaction at most, and hence for parent states below core-valence separation thresholds:

$$R(\alpha,\gamma,
u;r) \xrightarrow{r \to \infty} C(\alpha,\gamma,
u) \frac{W_{-\eta,l+1/2}(2kr)}{r},$$

where  $W_{-\eta,l+1/2}(2kr)$  is a Whitakker function with  $k = \sqrt{2\mu B}/\hbar$ , B is the separation energy, and  $C(\alpha, \gamma, \nu)$  is the asymptotic normalization coefficient or ANC.

GFMC evaluation of R is by extrapolation requiring two mixed estimates minus the VMC result:

 $R(\alpha,\gamma,\nu;r;\tau) \approx \langle R(\alpha,\gamma,\nu;r;\tau) \rangle_{M_A} + \langle R(\alpha,\gamma,\nu;r;\tau) \rangle_{M_{A-1}} - \langle R(\alpha,\gamma,\nu;r) \rangle_{V},$ 

where  $M_A$  denotes a mixed estimate where parent  $\Psi_A(\alpha; \tau)$  has been propagated in GFMC and  $M_{A-1}$  is a mixed estimate where daughter  $\Psi_{A-1}(\gamma; \tau)$  has been propagated.



Imaginary time evolution of overlaps in the  $p_{3/2}$  channel of the overlap  $\langle {}^{6}\text{He} + p | {}^{7}\text{Li} \rangle$ 

A convenient parametrization for input to PTOLEMY or other direct reaction code is provided by fitting a single-particle potential to reproduce the overlap R:

$$V(r) = V_{WS} \left[ \frac{1}{1 + \exp((r - R_{WS})/a_{WS})} - \beta \exp(-(r/\rho)^2) \right] + \left( 4\vec{l} \cdot \vec{s} \right) \frac{V_{so}}{r} \frac{d}{dr} \left[ \frac{1}{1 + \exp((r - R_{so})/a_{so})} \right] + V_{Coul}$$

The potential parameters are adjusted to minimize  $\chi^2$  under the constraint that the overlap tail falls off with the correct core-valence separation energy *B*. This helps in extraction of the ANCs.

Brida, Pieper, & Wiringa, in preparation

# Example: (<sup>3</sup>H,<sup>4</sup>He), s<sub>1/2</sub> overlap



# Example: (<sup>6</sup>He,<sup>7</sup>Li), p<sub>3/2</sub> overlap







# **GFMC** separation energies

٨	Λ 1	B [MeV]		
A	A-T	GFMC	ехр	
ЗН	<sup>2</sup> H	6.24	6.26	
³Не	<sup>2</sup> H	5.49	5.49	
<sup>4</sup> He	<sup>з</sup> Н	19.96	19.81	
	<sup>3</sup> Не	20.71	20.58	
<sup>7</sup> Li(g.s.)	<sup>6</sup> He(g.s)	9.88	9.98	
	<sup>6</sup> Li(g.s)	7.15	7.25	
	<sup>6</sup> Li(3+)	9.49	9.44	
	<sup>6</sup> Li(0+)	10.65	10.81	
<sup>7</sup> Li(1/2-)	<sup>6</sup> Li(g.s)	6.95	6.77	
<sup>7</sup> Be(g.s.)	<sup>6</sup> Li(g.s)	5.69	5.61	
	<sup>6</sup> Li(3+)	8.03	7.79	
	<sup>6</sup> Li(0+)	9.18	9.17	

- total energies are within 1% around exp. values
- sep. energies are within 3% around exp. values
- use exp. sep. energies for ANCs accounting for uncertainties

# s-shell: spectroscopic factors

А	Λ 1	channel -	S		
	A-T		GFMC	ехр	
ЗΗ	<sup>2</sup> H	S <sub>1/2</sub>	1.30		
		d <sub>3/2</sub>	0.0224		
<sup>3</sup> Не	2	S <sub>1/2</sub>	1.31		
	П	d <sub>3/2</sub>	0.0221		
<sup>4</sup> He –	<sup>3</sup> Н	S <sub>1/2</sub>	1.61	1.4-1.6	
	<sup>3</sup> He	S <sub>1/2</sub>	1.60		

GFMC systematic uncertainties are 2-3% or less exp. values: Pandharipande et al, RMP 69 (1997) 981

# s-shell: ANCs

A A-1	L channel –	ANC [fm <sup>-1/2</sup> ]			
		GFMC	exp		
		S <sub>1/2</sub>	2.14	2.11(3), 2.07(2), 1.87(14)	
<sup>3</sup> Н	$^{2}H$	<b>d</b> <sub>3/2</sub>	-0.0848		
		<i>d/s</i>	-0.0396	-0.0418(15)	
		S <sub>1/2</sub>	2.10	2.10(16), 1.76(11)	
<sup>з</sup> Не	$^{2}H$	<b>d</b>	-0.0762		
		d <sub>3/2</sub> /s <sub>1/2</sub>	-0.0363	-0.0389(42)	
<sup>4</sup> He —	<sup>3</sup> Н	S <sub>1/2</sub>	6.45	7.36(19), 6.70(50), 5.44(15)	
	<sup>з</sup> Не	S <sub>1/2</sub>	6.45	6.77(51), 6.52(49)	

GFMC systematic uncertainties are 5% or less exp. values: Timofeyuk (2010), Girard (1979), Locher (1978, Purcell (2010), Blimov (1985, Blokhintsev (1977)

# s-shell: comparing with HH



# p-shell: spectroscopic factors

А	A-1	channel -	S		
			GFMC	exp	
<sup>7</sup> Li(g.s.)	<sup>6</sup> He(g.s)	р <sub>3/2</sub>	0.406	0.44(6), 0.42(4)	
	<sup>6</sup> Li(g.s)	$p_{_{1/2}}$	0.230		
		$p_{_{3/2}}$	0.438		
		$\sum S$	0.668	0.74(11), 073(5)	
	<sup>6</sup> Li(3+)	р <sub>3/2</sub>	0.435	0.72(14), 0.58(13)	
	<sup>6</sup> Li(0+)	р <sub>3/2</sub>	0.203	0.19(3)	
<sup>7</sup> Li(1/2-)	<sup>6</sup> Li(g.s)	$p_{_{1/2}}$	0.060		
		$p_{_{3/2}}$	0.759		
		$\sum S$	0.819	1.15, 0.90(9)	

SFs for overlaps with <sup>7</sup>Be(g.s) are close to <sup>7</sup>Li(g.s) Shell-model SFs quenched by as much as 40%. GFMC systematic uncertainties are 2-3% or less exp. values: Wuosmaa (2008), Lapikas (1999), Ju (2010), Li (1969), Towner (1969), Schiffer (1967)

# p-shell: ANCs

^	A-1	channel —	ANC [fm <sup>-1/2</sup> ]		
A			GFMC	exp	
<sup>7</sup> Li(g.s.)	<sup>6</sup> He(g.s)	$p_{_{3/2}}$	3.52	2.48	
	<sup>6</sup> Li(g.s)	$p_{_{1\!/\!2}}$	1.73		
		$p_{_{3/2}}$	2.29		
		$\sqrt{\sum ANC^2}$	<sup>2</sup> 2.87	1.26-2.82	
	<sup>6</sup> Li(3+)	$p_{_{3/2}}$	3.50	2.06-3.00	
	<sup>6</sup> Li(0+)	$p_{_{3/2}}$	2.39	1.71-2.62	
<sup>7</sup> Li(1/2-)	<sup>6</sup> Li(g.s)	$p_{_{1\!/\!2}}$	0.57		
		$p_{_{3/2}}$	2.85		
		$\sqrt{\sum ANC^2}$	<sup>2</sup> 2.91		

ANCs for overlaps with <sup>7</sup>Be(g.s) are close to <sup>7</sup>Li(g.s) GFMC systematic uncertainties are 5% or less exp. values: Gulamov (1995), Bekbaev (1991)

### ALTERNATE ROUTE TO ANCS

The VMC wave functions account fairly well for short-range correlations but may have poor asymptotic behavior, particularly in p-shell.

Fitting C = rR(r)/W(2kr) is generally difficult because long-range shapes can be wrong, and Monte Carlo sampling of the tails is difficult.

In the s-shell, however, it works ok:



#### INTEGRAL REALTION FOR THE ANC

There is a better way than explicit overlaps, ideally suited to QMC methods

Consider the A-body wave function  $\Psi_A$  and its overlap with  $\Psi_{A-1}$  plus a final proton with separation energy B.

Write the Schrödinger equation as

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

and expand H and E into parts internal to  $\Psi_{A-1}$  and parts involving the last particle

$$\left(H_{\text{int}} + T_{\text{rel}} + U_{\text{rel}} + V_C - V_C - E_{\text{int}} + B\right)\Psi_A = 0$$

Then

$$\Psi_A = -[T_{\rm rel} + V_C + B]^{-1} (U_{\rm rel} - V_C) \Psi_A -[T_{\rm rel} + V_C + B]^{-1} (H_{\rm int} - E_{\rm int}) \Psi_A$$

The second line is zero since  $(H_{int} - E_{int})\Psi_{A-1} = 0$ 

Rewriting the Green's function  $[T_{rel} + V_C + B]^{-1}$  in terms of special functions turns

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

into

$$\Psi_{A-1}^{\dagger}\chi^{\dagger}Y_{lm}^{\dagger}\Psi_{A} = \frac{2\mu}{k\hbar^{2}w}\mathcal{A}\int \frac{M_{-\eta,l+\frac{1}{2}}(2kr_{<})W_{-\eta,l+\frac{1}{2}}(2kr_{>})}{r_{<}r_{>}}$$
$$\times\Psi_{A-1}^{\dagger}\chi^{\dagger}Y_{lm}^{\dagger}(\mathbf{\hat{r}}_{cc})\left(U_{rel}-V_{C}\right)\Psi_{A}d\mathbf{R}$$

so at large radius

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

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

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

and at large separation of the last nucleon,  $U_{rel} \rightarrow V_C$ , so  $(U_{rel} - V_C) \rightarrow 0$ . This makes the integrand terminate at  $\sim 7$  fm for AV18+UIX.

This is great for QMC methods, which are good at integration over the wave function interior, but bad in the tails.

ANC: <sup>3</sup>He  $\rightarrow dp$ 



Points are Monte-Carlo sampled integrand; solid curves are cumulative integrals For <sup>3</sup>He  $\rightarrow dp$ , we get  $C_s^{dp} = 2.131(8) \text{ fm}^{-1/2}$ ,  $C_d^{dp} = -0.0927(10) \text{ fm}^{-1/2}$ Corresponding HH values are 2.16 & -0.0865Corresponding GFMC values are 2.10 & -0.0794

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

### ANC: <sup>8</sup>Li $\rightarrow$ <sup>7</sup>Li + n

Here is a case where fitting to VMC samples is impossible, but the integral method using the laboratory separation energy works beautifully:



ANC ( $fm^{-1}$ )	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)

### Results for one-nucleon removal $3 \leq A \leq 9$



- 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 few exceptions, these are the first *ab initio* ANCs in A > 4

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

### QMC FOR CONTINUUM STATES

We generally treat nuclei as particle-stable systems – probably good for energies of narrow resonances, but no prediction for widths. For wide states we need full scattering solution.

#### METHOD

- Pick a logarithmic derivative,  $\chi$ , at some large boundary radius ( $R_B \approx 9 \text{ fm}$ )
- GFMC propagation, using method of images to preserve  $\chi$  at R, finds  $E(R_B, \chi)$
- Phase shift,  $\delta(E)$ , is function of  $R_B$ ,  $\chi$ , E
- Repeat for a number of  $\chi$  until  $\delta(E)$  is mapped out
- need E accurate to  $\sim 1/3\%$



### <sup>5</sup>He as $n+^4$ He scattering

Black curves: Hale phase shifts from *R*-matrix analysis up to  $J = \frac{9}{2}$  of data AV18 with no  $V_{ijk}$  underbinds <sup>5</sup>He(3/2<sup>-</sup>) & overbinds <sup>5</sup>He(1/2<sup>-</sup>) AV18+UIX improves <sup>5</sup>He(1/2<sup>-</sup>) but still too small spin-orbit splitting AV18+IL2 reproduces locations and widths of both *P*-wave resonances



Nollett, Pieper, Wiringa, Carlson, & Hale, PRL 99, 022502 (2007)

### WIDTHS AS ANCS

Mapping  $E(\gamma) \to \delta(E)$  is laborious, requires many solutions, and sensitive to calculational precision Reliable widths of narrow states will be difficult by this method

But 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 ( $\delta = 90^\circ$ ; 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  $|C_{lj}|^2 v = \frac{\hbar k}{\mu} |C_{lj}|^2$ 

From  $\Gamma \simeq \hbar/\tau$ , we get  $\Gamma \simeq \frac{\hbar^2 k}{\mu} |C_{lj}|^2$ 

One could also consider Gamow's decaying complex-energy states and getthe 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

You can get from one to the other by considering the bound k and  $\eta$  as  $\pm i$  times their scattering-state counterparts

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  $\alpha$  and p decays (e.g. Esbensen & Davids (2000) deformed proton emitters)

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

The integral estimate should apply to states that are in some sense narrow Here are low-lying states in  $A \le 9$  with width mainly/all in nucleon emission



Nollett & Wiringa, in preparation

Lots of widths come out close to experiment

Widths not close to experiment generally have some unaccounted-for width (e.g.  $\alpha$  or 3-body channel) or isospin mixing, or are broad

Pseudobound <sup>5</sup>He states yield wildly unreasonable widths, probably because they're very broad

Width integral appears to be better than just using the Wigner limit and  $S_{lj}$ 

### FUTURE WORK

GFMC one-nucleon overlaps for  $A \ge 8$  nuclei

Two-nucleon overlaps like  $\langle \alpha nn | {}^{6}\text{He} \rangle$  and  $\langle \alpha d | {}^{6}\text{Li} \rangle$  under development – first VMC calculations made

Generalize integral method for ANCs and widths to  $\alpha$  and other cluster breakups

Utilize integral method with GFMC wave functions and IL7 potential

Integral method may provide way of extracting surface amplitudes from GFMC for coupled-channel scattering problems

Still need to do full scattering calculations for wide states like  ${}^{8}\text{Be}(2^{+}, 4^{+})$  but integral method will probably give best estimate of width of  ${}^{8}\text{Be}(0^{+})$ 

# Example: 2N overlaps for <sup>6</sup>He

### 2N overlaps in the past:

three-body calculations

- 3-body w.f.s are the 2N overlaps
- inert core, simple interactions, ...
- microscopic calculations
  - I.Brida and F.M.Nunes, NPA 847(2010) 1
     phenomenological N-N forces
  - spec. factors greater by 30%-70% than in 3-body

10

10

10<sup>6</sup> [10<sup>6</sup> 10<sup>6</sup> 10<sup>6</sup>

-10

5

10 [fm]

0



K=6, d-waves K=6, f-waves

15

20

0.6

### **Present:**

VMC:

- fully ab-initio
- preliminary VMC results:

# Future:

