Nuclear quantum Monte Carlo

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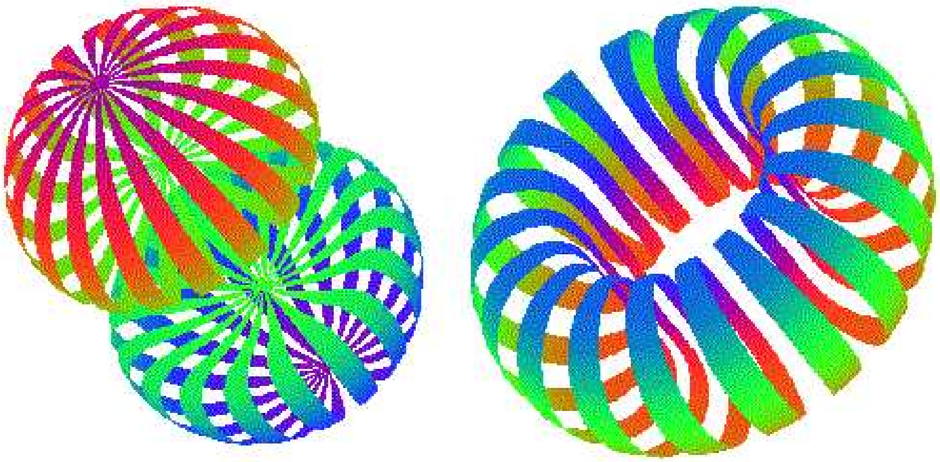


Work not possible without extensive computer resources

Argonne Laboratory Computing Resource Center (Jazz & Fusion)
Argonne Math. & Comp. Science Division (BlueGene/L & SiCortex)
Argonne Leadership Computing Facility (Intrepid & Mira)

Argonne NATIONAL LABORATORY

Physics Division

Work supported by U.S. Department of Energy, Office of Nuclear Physics

Ab Initio Calculations of Light Nuclei

Goals

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

- Binding energies, excitation spectra, relative stability
- Densities, electromagnetic moments, transition amplitudes, cluster-cluster overlaps
- Low-energy NA & AA' scattering, asymptotic normalizations, astrophysical reactions

Requirements

- Two-nucleon potentials that accurately describe elastic NN scattering data
- Consistent three-nucleon potentials and electroweak current operators
- Accurate 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 $A \leq 12$ nuclei in good agreement with experiment
- Applications to elastic & ineleastic e, π scattering, $(e, e'p)$, (d, p) reactions, etc.
- Electromagnetic moments, $M1$, $E2$, F, GT transitions calculated
- ^{5}He = $n\alpha$ scattering and $3 \leq A \leq 9$ ANCs and widths

NUCLEAR HAMILTONIAN

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

$$K_i = -\frac{\hbar^2}{4}[(\frac{1}{m_p} + \frac{1}{m_n}) + (\frac{1}{m_p} - \frac{1}{m_n})\tau_{iz}]\nabla_i^2$$

Argonne v_{18}

Wiringa, Stoks, & Schiavilla, PRC **51**, 38 (1995)

$$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij})O_{ij}^p$$

v_{ij}^{γ}: pp, pn & nn electromagnetic terms

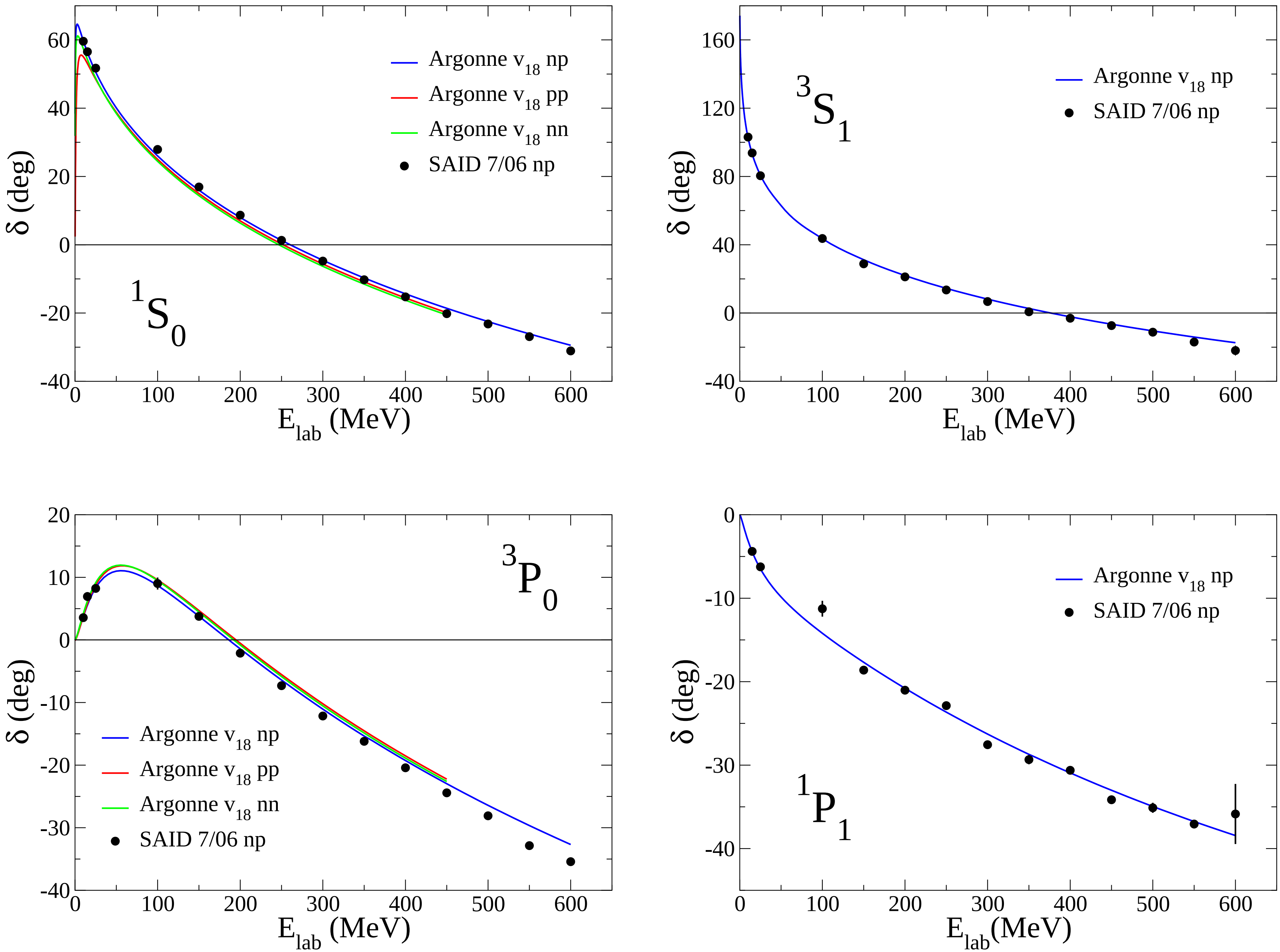
$$v_{ij}^{\pi} \sim [Y_\pi(r_{ij})\sigma_i \cdot \sigma_j + T_\pi(r_{ij})S_{ij}] \otimes \tau_i \cdot \tau_j$$

$$v_{ij}^{I} = \sum_p I^p T_\pi^2(r_{ij})O_{ij}^p$$

$$v_{ij}^{S} = \sum_p [P^p + Q^p r + R^p r^2]W(r)O_{ij}^p$$

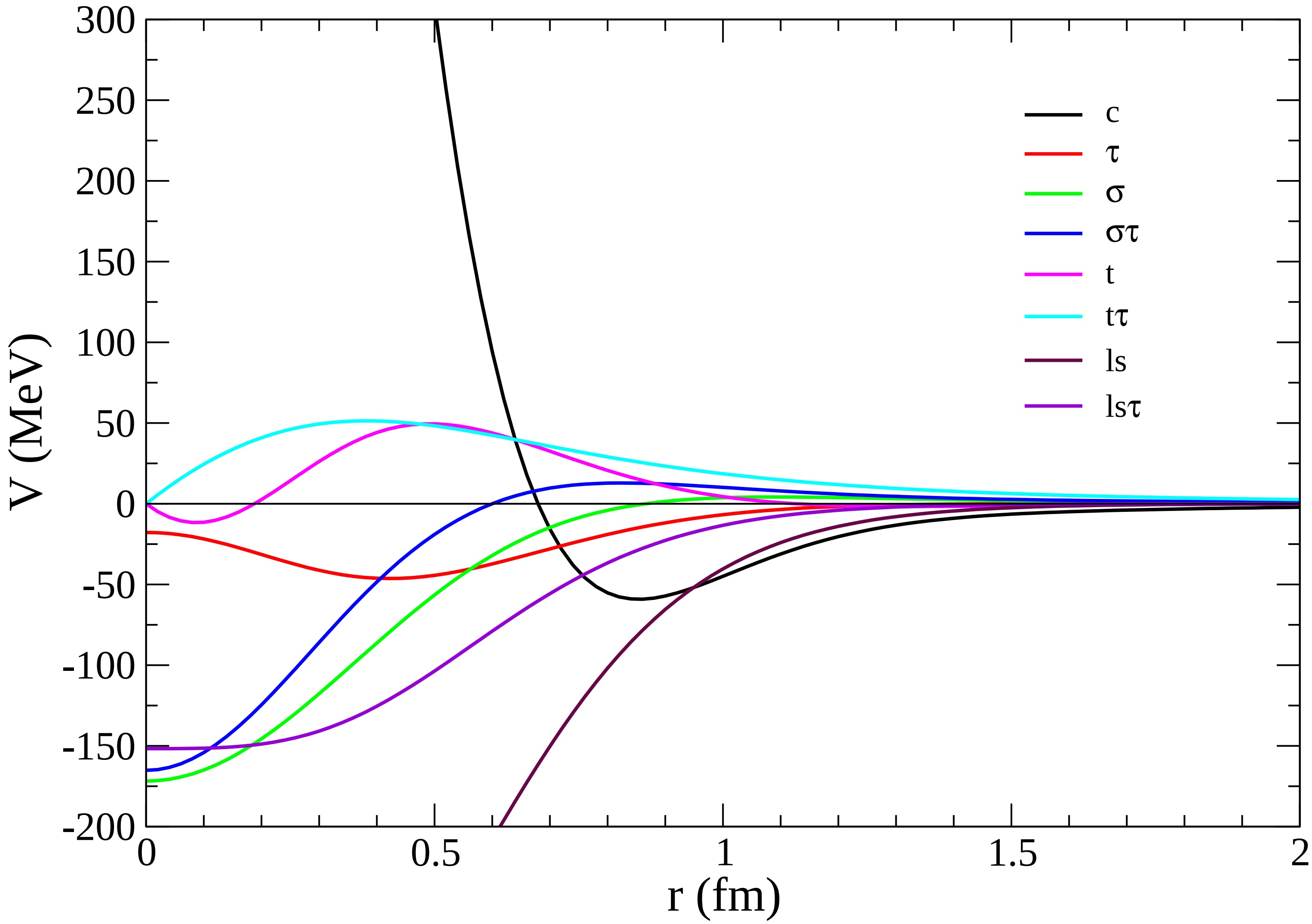
$$\begin{aligned} O_{ij}^p = & [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2(\sigma_i \cdot \sigma_j), (\mathbf{L} \cdot \mathbf{S})^2] \\ & + [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2(\sigma_i \cdot \sigma_j), (\mathbf{L} \cdot \mathbf{S})^2] \otimes \tau_i \cdot \tau_j \\ & + [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}] \otimes T_{ij} \\ & + [1, \sigma_i \cdot \sigma_j, S_{ij}, \mathbf{L} \cdot \mathbf{S}] \otimes (\tau_i + \tau_j)_z \end{aligned}$$

$$S_{ij} = 3\sigma_i \cdot \hat{r}_{ij}\sigma_j \cdot \hat{r}_{ij} - \sigma_i \cdot \sigma_j \qquad T_{ij} = 3\tau_{iz}\tau_{jz} - \tau_i \cdot \tau_j$$



Argonne v_{18} fits Nijmegen PWA93 data base of 1787 *pp* & 2514 *np* observables for $E_{lab} \leq 350$ MeV with χ^2/datum = 1.1 plus *nn* scattering length & ^{2}H binding energy

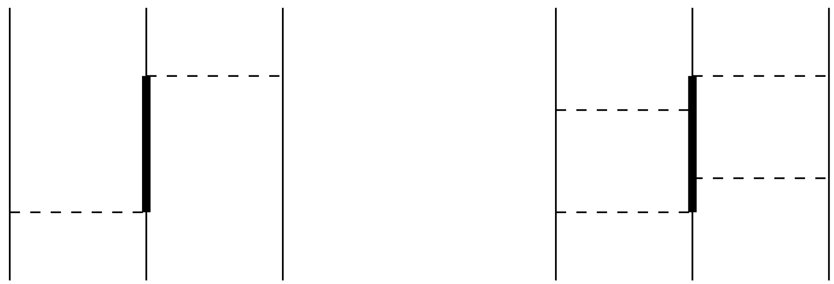
Argonne v_{18}



Uses 42 I^p, P^p, Q^p, R^p parameters [constrained so that $v_t(r=0) = 0$ & $\frac{\partial v_{p\neq t}}{\partial r}|_{r=0} = 0$] plus $f_{\pi NN}$ coupling strength & one cutoff parameter in $Y_\pi(r)$, $T_\pi(r)$.

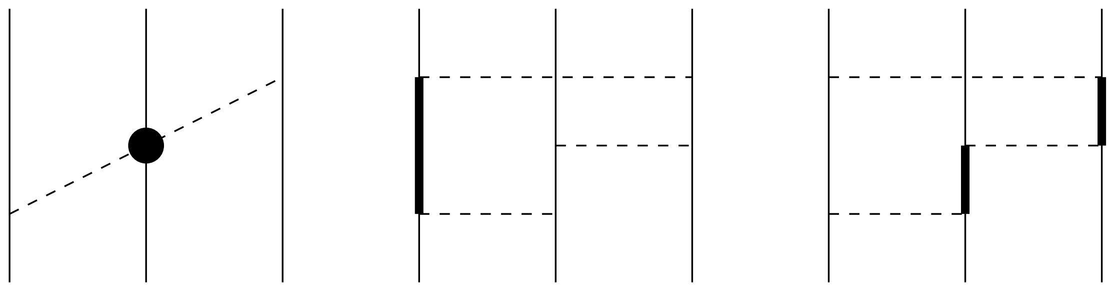
THREE-NUCLEON POTENTIALS

Urbana $V_{ijk} = V^{2\pi P}_{ijk} + V^{R}_{ijk}$



Carlson, Pandharipande, & Wiringa, NP **A401**, 59 (1983)

Illinois $V_{ijk} = V^{2\pi P}_{ijk} + V^{2\pi S}_{ijk} + V^{3\pi \Delta R}_{ijk} + V^{R}_{ijk}$



Pieper, Pandharipande, Wiringa, & Carlson, PRC **64**, 014001 (2001)

Illinois-7 has 4 strength parameters fit to 23 energy levels in $A \leq 10$ nuclei.

In light nuclei we find (thanks to large cancellation between $\langle K \rangle$ & $\langle v_{ij} \rangle$):

$$\langle V_{ijk} \rangle \sim (0.02 \text{ to } 0.07)\ \langle v_{ij} \rangle \sim (0.15 \text{ to } 0.5)\ \langle H \rangle$$

We expect $\langle \mathcal{V}_{ijkl} \rangle \sim 0.05\ \langle V_{ijk} \rangle \sim (0.01 \text{ to } 0.03)\ \langle H \rangle \sim 1$ MeV in ^{12}C .

VARIATIONAL MONTE CARLO

Minimize expectation value of H

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0$$

using MeT^{2}R^{2}opolis Monte Carlo and trial function

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

- single-particle $\Phi_A(JMTT_3)$ is fully antisymmetric and translationally invariant
- central pair correlations $f_c(r)$ keep nucleons at favorable pair separation
- pair correlation operators $U_{ij} = \sum_p u_p(r_{ij}) O^p_{ij}$ reflect influence of v_{ij}
- triple correlation operator U_{ijk} added when V_{ijk} is present
- multiple J^π states constructed and diagonalized for p-shell nuclei
- ability to construct clusterized or asymptotically correct trial functions

Ψ_V are spin-isospin vectors in $3A$ dimensions with $\sim 2^A \binom{A}{Z}$ components

Lomnitz-Adler, Pandharipande, & Smith, NP **A361**, 399 (1981)
Wiringa, PRC **43**, 1585 (1991)

Scaling of VMC calculation time with nucleus

Scales with # particles (6A w.f. calculations for kinetic energy) $\times$
pairs (operations to construct w.f.) $\times$ spin$\times$isospin (size of w.f. vector):

	A	Pairs	Spin$\times$Isospin	$\prod(/^{8}\mathrm{Be})$
^{4}He	4	6	16$\times$2	0.001
^{5}He	5	10	32$\times$5	0.010
^{6}Li	6	15	64$\times$5	0.036
^{7}Li	7	21	128$\times$14	0.33
^{8}Be	8	28	256$\times$14	1.
^{9}Be	9	36	512$\times$42	8.7
^{10}Be	10	45	1024$\times$90	52.
^{11}B	11	55	2048$\times$132	200.
^{12}C	12	66	4096$\times$132	530.
^{14}C	14	91	16384$\times$1001	26,000.
^{16}O	16	120	65536$\times$1430	220,000.
^{40}Ca	40	780	$1.1\times10^{12} \times 6.6\times10^{9}$	2.8×10^{20}
^{8}n	8	28	256$\times$1	0.071
^{16}n	16	120	65536$\times$1	160.

GREEN'S FUNCTION MONTE CARLO

Projects out lowest energy state from variational trial function

$$\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau] a_n \psi_n$$

$$\Psi(\tau \to \infty) = a_0 \psi_0$$

Evaluation of $\Psi(\tau)$ done stochastically in small time steps $\Delta\tau$

$$\Psi(\mathbf{R}_n, \tau) = \int G(\mathbf{R}_n, \mathbf{R}_{n-1}) \cdots G(\mathbf{R}_1, \mathbf{R}_0) \Psi_V(\mathbf{R}_0) d\mathbf{R}_{n-1} \cdots d\mathbf{R}_0$$

Mixed estimates used for expectation values

$$\langle O(\tau) \rangle = \frac{\langle \Psi(\tau)|O|\Psi(\tau)\rangle}{\langle \Psi(\tau)|\Psi(\tau)\rangle} \approx \langle O(\tau)\rangle_{\mathrm{Mixed}} + [\langle O(\tau)\rangle_{\mathrm{Mixed}} - \langle O \rangle_V]$$

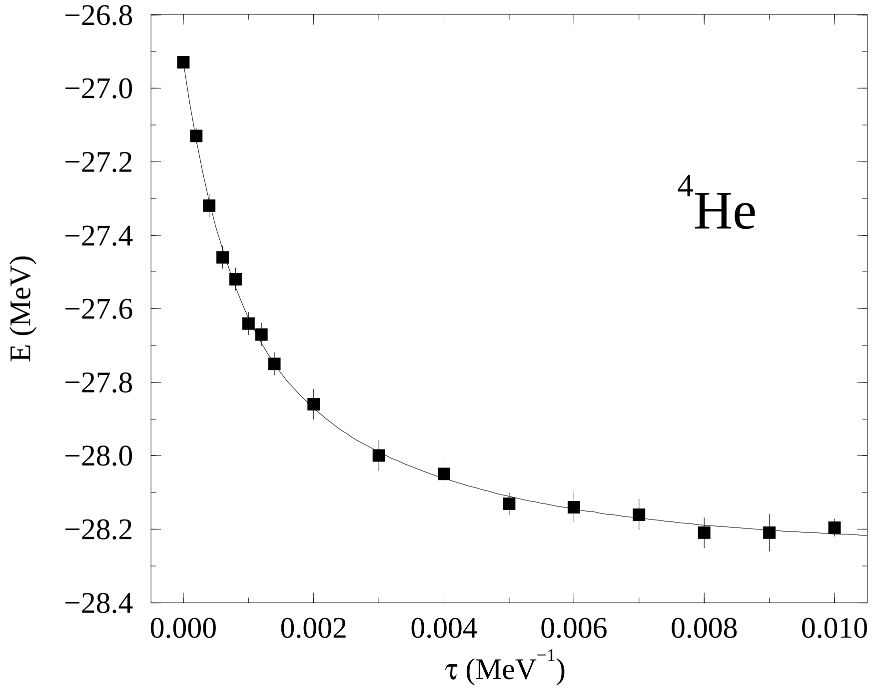
$$\langle O(\tau)\rangle_{\mathrm{Mixed}} = \frac{\langle \Psi_V|O|\Psi(\tau)\rangle}{\langle \Psi_V|\Psi(\tau)\rangle} \quad ; \quad \langle H(\tau)\rangle_{\mathrm{Mixed}} = \frac{\langle \Psi(\tau/2)|H|\Psi(\tau/2)\rangle}{\langle \Psi(\tau/2)|\Psi(\tau/2)\rangle} \geq E_0$$

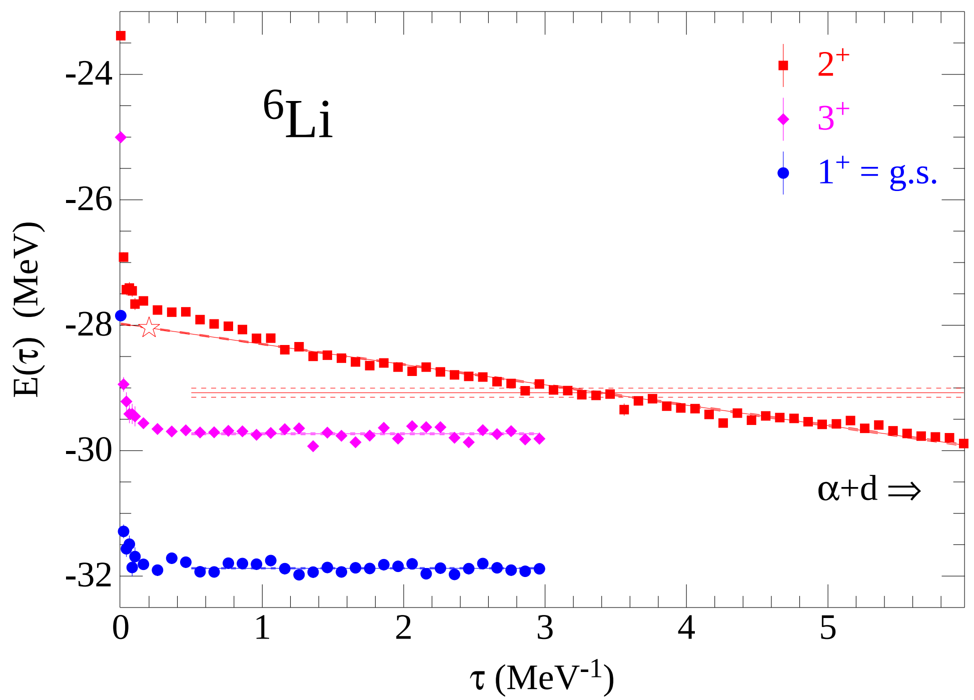
- Cannot propagate p^2, L^2, or $(\mathbf{L}\cdot\mathbf{S})^2$ operators $\Rightarrow$ use H' = AV8′ + $\tilde{V}_{ijk}$
- Fermion sign problem would limit maximum τ, but ...
- Constrained-path propagation removes steps that have $\overline{\Psi^\dagger(\tau,\mathbf{R})\Psi_V(\mathbf{R})} = 0$
- Multiple excited states of same J^π stay orthogonal

Pudliner, Pandharipande, Carlson, Pieper, & Wiringa, PRC **56**, 1720 (1997)

Wiringa, Pieper, Carlson, & Pandharipande, PRC **62**, 014001 (2000)

EXAMPLES OF GFMC PROPAGATION





- Curve has $\sum_i a_i \exp(-E_i\tau)$ with E_i = 1480, 340 & 20.2 MeV (20.2 MeV is first ^{4}He 0^+ excitation)
- Ψ_V has small amounts of 1.5 GeV contamination

- g.s. (1^+) & 3^+ stable after τ = 0.2 MeV^{-1}
  2^+ (a broad resonance) never stable – decaying to separated α & d
- $E(\tau$=0.2) is best GFMC estimate of resonance energy

GFMC FOR SECOND EXCITED STATES OF SAME J^π

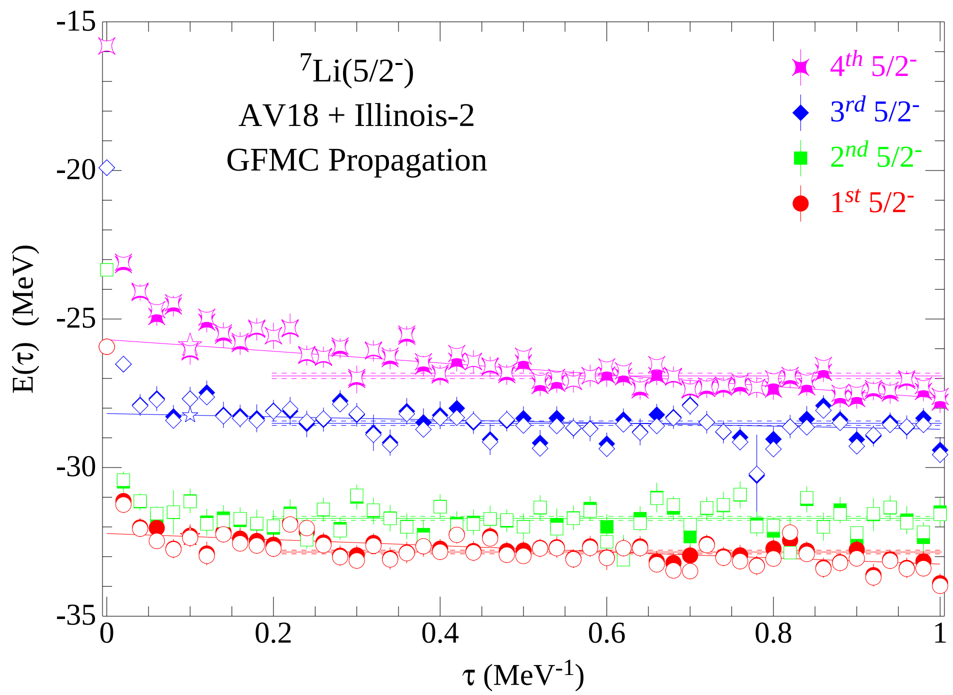
The Ψ_V are constructed by non-orthogonal basis diagonalization in p-shell wave functions.

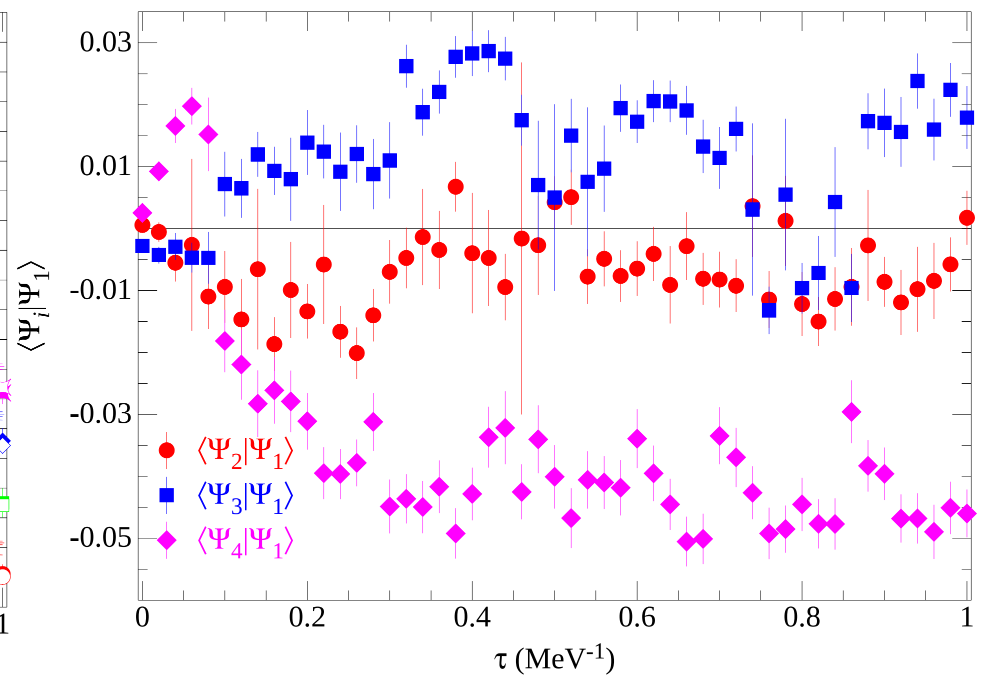
Example: ^{7}Li(5/2-) has 4 symmetry possibilities: ^{2}F[43] , ^{4}P[421] , ^{4}D[421] , ^{2}D[421]

$\langle \Psi_V(2^{nd}\frac{5}{2}^-) | \Psi_V(1^{st}\frac{5}{2}^-) \rangle = 0$, but $\langle \Psi_{\text{GFMC}}(2^{nd}\frac{5}{2}^-) | \Psi_V(1^{st}\frac{5}{2}^-) \rangle$ need not be zero.

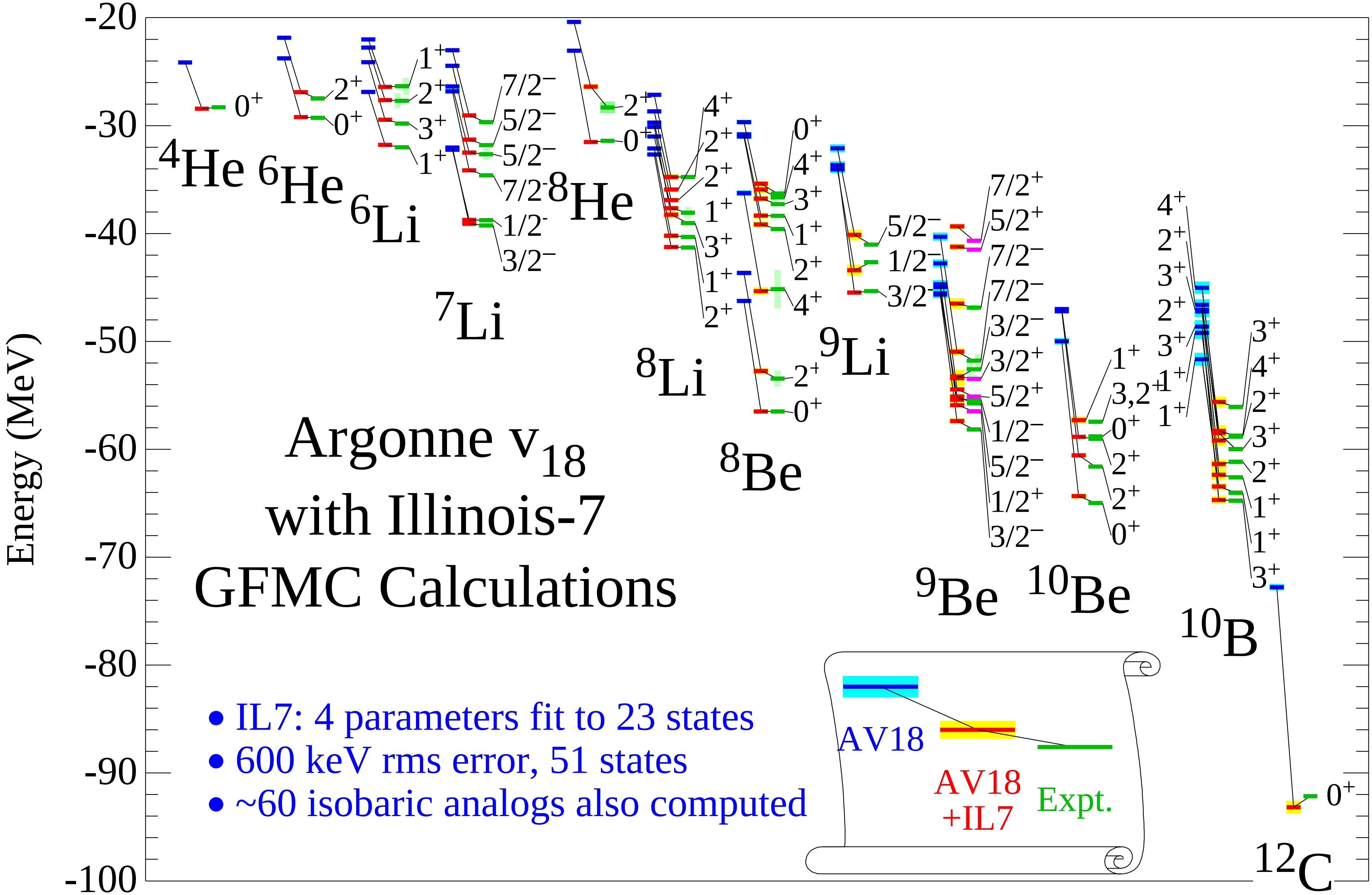
Will $e^{-(H-\tilde{E}_0)\tau}\Psi_V(2^{nd}\frac{5}{2}^-) \rightarrow \Psi_{\text{GFMC}}(1^{st}\frac{5}{2}^-)$?

Can use $\langle \Psi_{\text{GFMC}}(i) | H | \Psi_{\text{GFMC}}(j) \rangle$ and $\langle \Psi_{\text{GFMC}}(i) | \Psi_{\text{GFMC}}(j) \rangle$ to rediagonalize

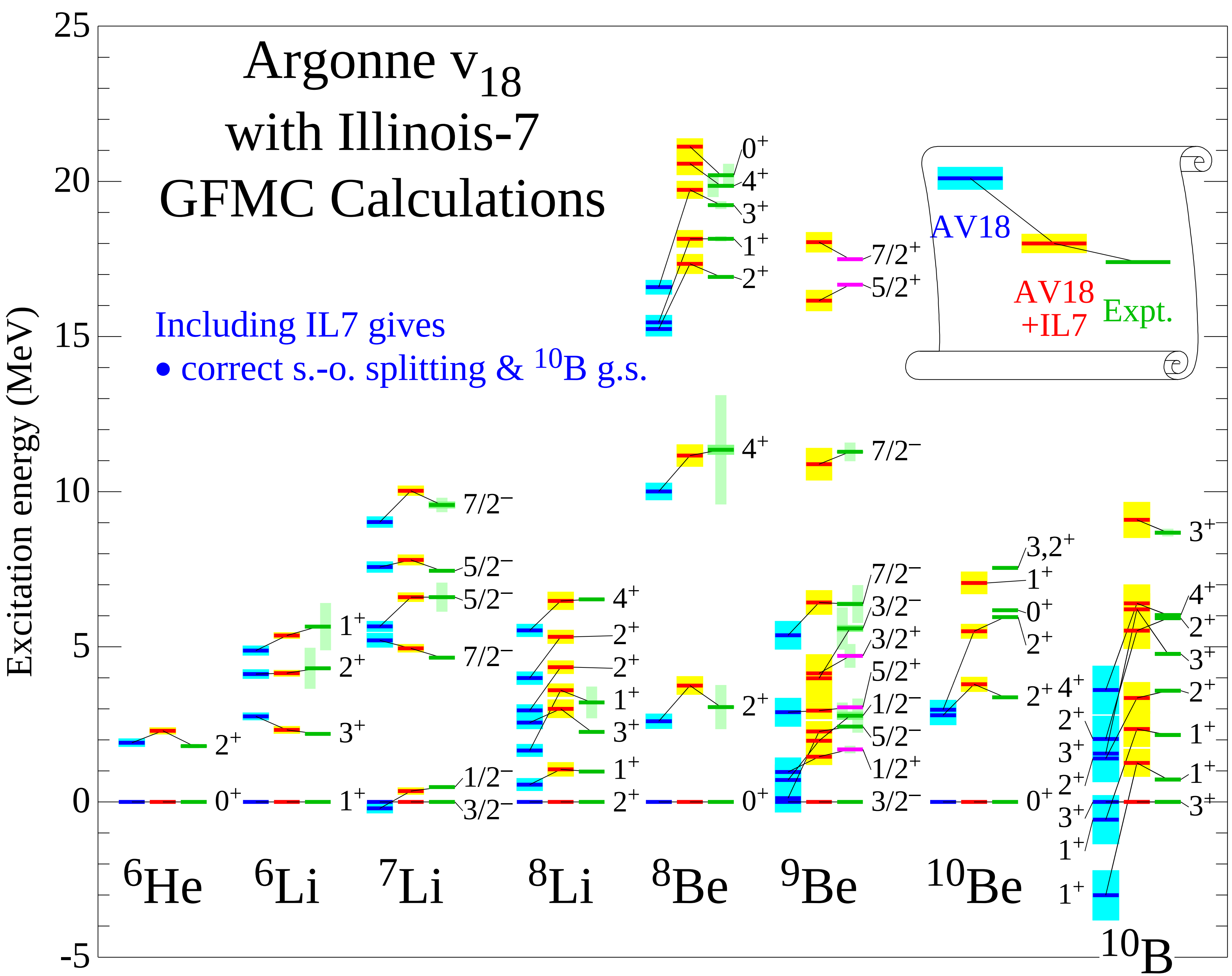




Pieper, Wiringa, & Carlson, Phys. Rev. C **70**, 054325 (2004)



Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C
Argonne v18
with Illinois-7
GFMC Calculations
• IL7: 4 parameters fit to 23 states
• 600 keV rms error, 51 states
• ~60 isobaric analogs also computed
AV18
AV18
+IL7
Expt.



Argonne v18
with Illinois-7
GFMC Calculations
Including IL7 gives
• correct s.-o. splitting & 10B g.s.
AV18
AV18
+IL7
Expt.
Excitation energy (MeV)
25
20
15
10
5
0
-5
6He
6Li
7Li
8Li
8Be
9Be
10Be
10B

1^{st} AND 2^{nd} (HOYLE) 0^+ STATES IN ^{12}C

Constructing the Jastrow part of the trial wave function is major effort:

- There are 5 LS-basis J=0^+ states in ^{12}C in the $0P$ shell:
  ^{1}S[444], ^{3}P[4431], ^{1}S[4422], ^{5}D[4422], ^{3}P[4332]
- All can be constructed by projections from a closed $(p3/2)^8$ shell (Carlson)
- Dominant 3-α symmetry is easily constructed with one α in the $0S$ shell and two αs in the $0P$ shell (Pandharipande)
- Additional components generated by promoting one whole α to the $1S$-$0D$ shell, and also promoting pairs, e.g., $0P^2 0D^2$ and $0P^2 1S^2$
- Total of 11 Jastrow components (some with considerable overlap) to be diagonalized

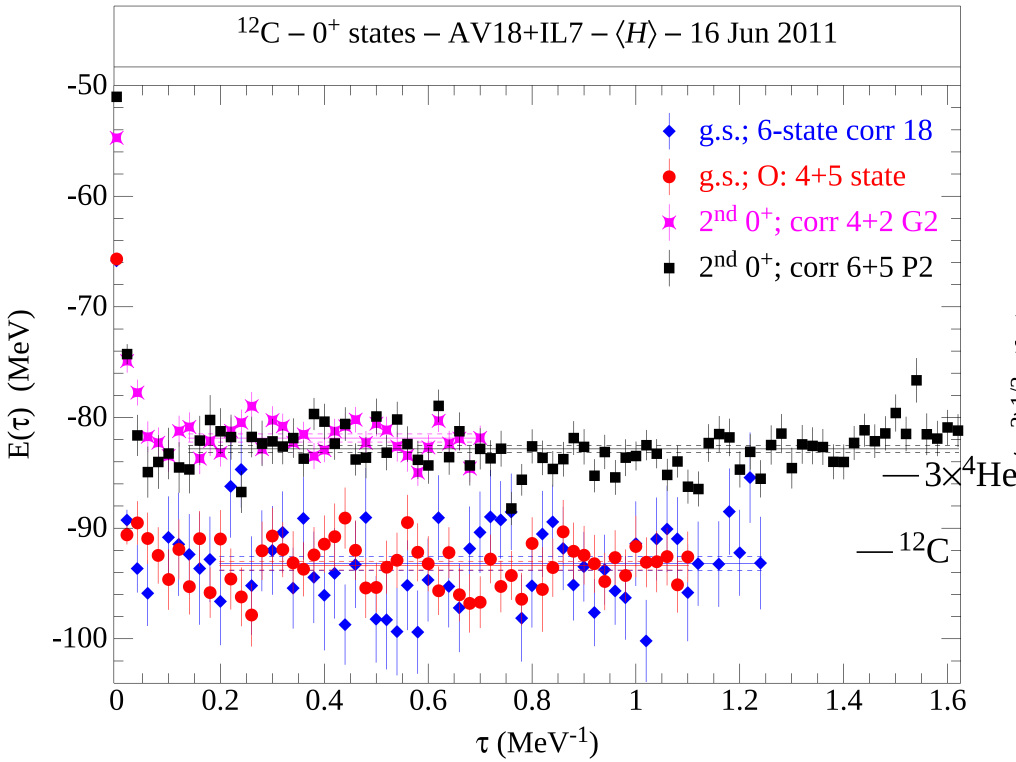
Challenge in GFMC propagation is keeping the 2^{nd} state orthogonal to the ground state

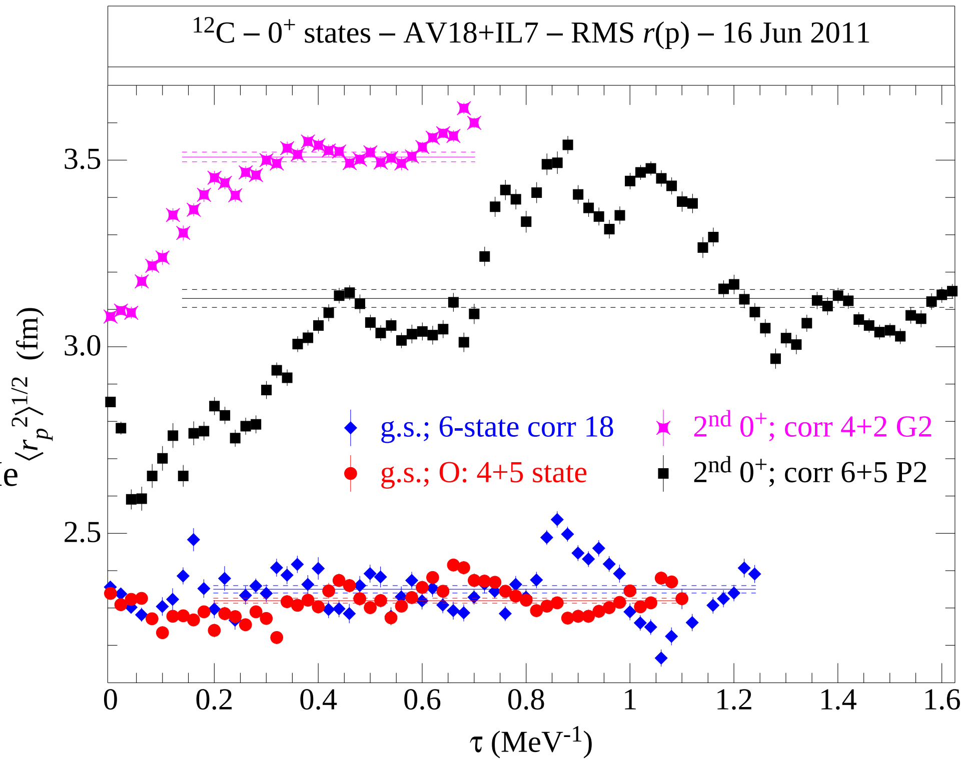
UNEDF SciDAC grant to develop general-purpose load-balancing library (ADLB) to run under MPI on 32,768 nodes with OpenMP for 4 cores/node

INCITE grant of Argonne's IBM BlueGene/P time used for calculations

1^{st} AND 2^{nd} (HOYLE) 0^+ STATES IN ^{12}C – PRELIMINARY

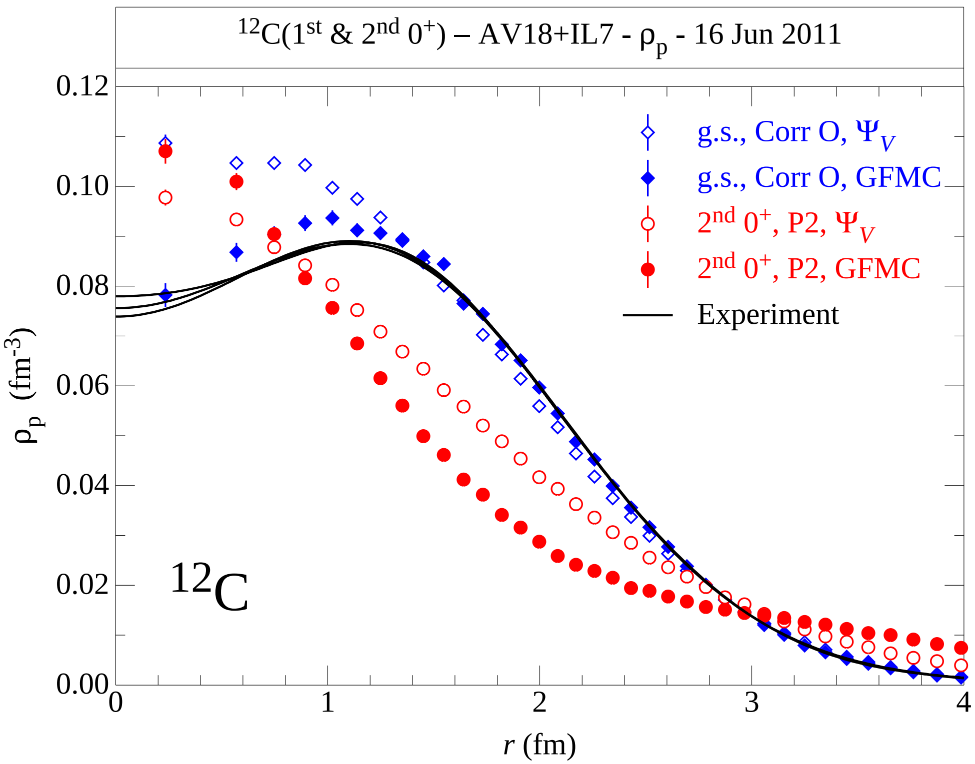
Convergence as a function of imaginary time (τ)

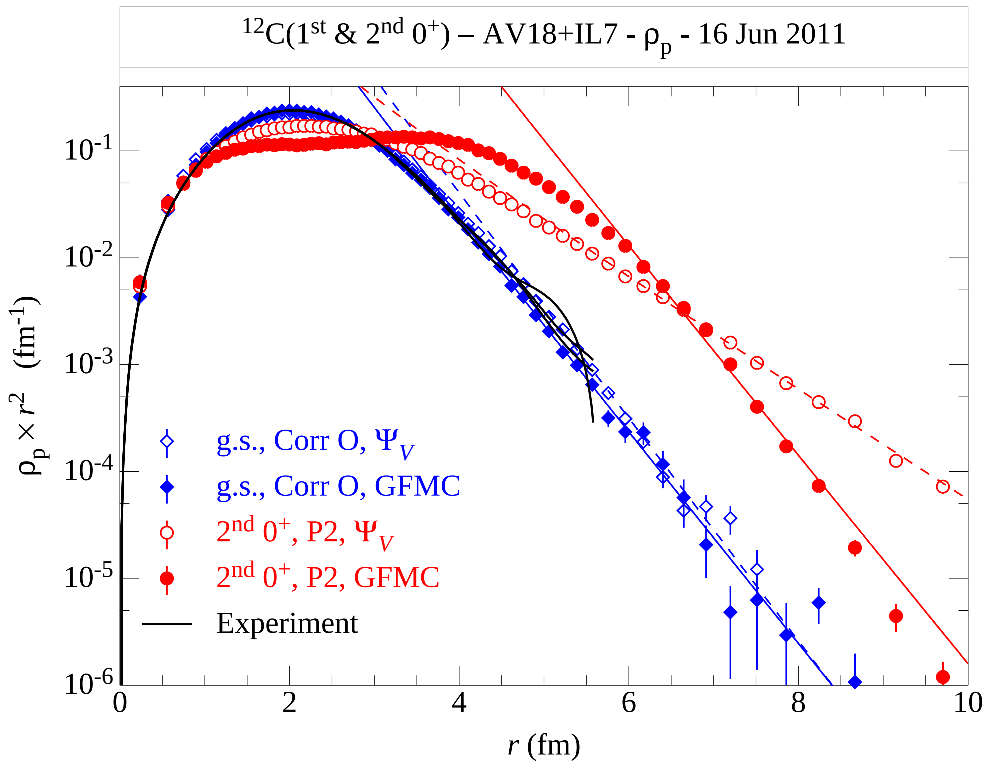




	g.s. energy			2^{nd} 0^+ E^*		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18	–44.9(2)	–73.2(5)		10.0(3)	7.9(6)	
AV18+IL7	–65.7(2)	–93.3(4)	–92.16	14.7(2)	10.4(5)	7.65

1^{st} AND 2^{nd} (HOYLE) 0^+ STATES IN ^{12}C – PRELIMINARY





Central density dip for ground state may be interpreted as three α's in a triangle

Central density peak for Hoyle state may be evidence for a linear configuration of three α's

Lusk, Pieper, & Butler, SciDAC Review Spring 2010

Nolen-Schiffer Anomaly

Nuclear forces are mostly charge-independent [CI $\propto 1, \tau_i \cdot \tau_j$], but have small charge-dependent [CD $\propto T_{ij}$] and charge-symmetry-breaking [CSB $\propto (\tau_i + \tau_j)_z$] components, while electromagnetic forces are a mix of CI, CD, & CSB terms. Evidence for strong charge-independence-breaking (CIB) comes from the energy differences of isobaric multiplets:

$$E_{A,T}(T_z) = \sum_{n \leq 2T} a_n(A,T) Q_n(T,T_z)$$

$$Q_0 = 1 \,;\, Q_1 = T_z \,;\, Q_2 = \tfrac{1}{2}(3T_z^2 - T^2)$$

For example,

$$a_1(3,\tfrac{1}{2}) = E(^3\mathrm{He}) - E(^3\mathrm{H})$$

$$a_2(6,1) = \tfrac{1}{3}[E(^6\mathrm{Be}) - 2E(^6\mathrm{Li}^*) + E(^6\mathrm{He})]$$

The Nolen-Schiffer anomaly is the difference not explained by Coulomb force; strong CIB and other electromagnetic terms in Argonne v_{18} explain the remainder (shown in keV):

$a_n(A,T)$	K^{CSB}	$v_{C1}(pp)$	$v^{\gamma,R}$	v^{CSB}+v^{CD}	Total	Expt.
$a_1(3,\frac{1}{2})$	14	647(0)	27	65(0)	753(0)	764
$a_1(7,\frac{1}{2})$	23	1457(3)	34	85(1)	1599(4)	1645
$a_2(6,1)$		166(0)	19	104(3)	289(4)	224
$a_2(8,1)$		137(1)	4	$-10(8)$	132(8)	145

Wiringa, AIP CP **1128**, 1 (2009)

Isospin-mixing in ^{8}Be

Experimental energies of 2^+ states

E_a = 16.626(3) MeV Γ_a^α = 108.1(5) keV

E_b = 16.922(3) MeV Γ_b^α = 74.0(4) keV

Isospin mixing of 2^+;1 and 2^+;0* states due to isovector interaction H_{01}:

$\Psi_a = \beta\Psi_0 + \gamma\Psi_1$; $\Psi_b = \gamma\Psi_0 - \beta\Psi_1$

decay through $T = 0$ component only

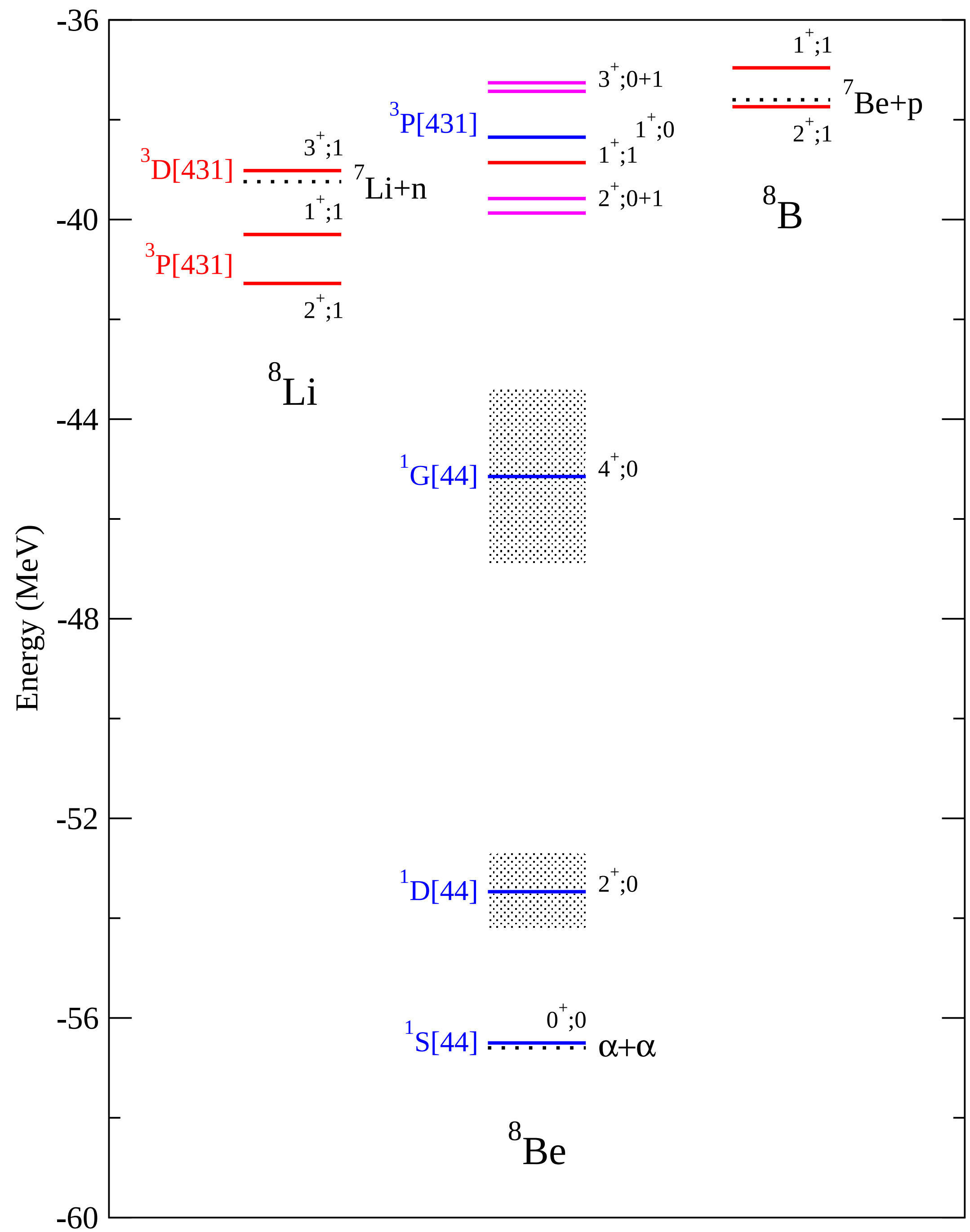
$\Gamma_a^\alpha/\Gamma_b^\alpha = \beta^2/\gamma^2 \Rightarrow \beta = 0.77$; $\gamma = 0.64$

$$E_{a,b} = \frac{H_{00} + H_{11}}{2} \pm \sqrt{\left(\frac{H_{00} - H_{11}}{2}\right)^2 + (H_{01})^2}$$

$H_{00} = 16.746(2)$ MeV

$H_{11} = 16.802(2)$ MeV

$H_{01} = -145(3)$ keV



GFMC mixed estimates for off-diagonal matrix elements

$$\frac{\langle\Psi^f(\tau)|O|\Psi^i(\tau)\rangle}{\sqrt{\langle\Psi^f(\tau)|\Psi^f(\tau)\rangle}\sqrt{\langle\Psi^i(\tau)|\Psi^i(\tau)\rangle}} \approx \langle O(\tau)\rangle_{M_i} + \langle O(\tau)\rangle_{M_f} - \langle O\rangle_V \ ,$$

where

$$\langle O\rangle_V = \frac{\langle\Psi^f_V|O|\Psi^i_V\rangle}{\sqrt{\langle\Psi^f_V|\Psi^f_V\rangle}\sqrt{\langle\Psi^i_V|\Psi^i_V\rangle}} \ ,$$

$$\langle O(\tau)\rangle_{M_i} = \frac{\langle\Psi^f_V|O|\Psi^i(\tau)\rangle}{\langle\Psi^i_V|\Psi^i(\tau)\rangle}\sqrt{\frac{\langle\Psi^i_V|\Psi^i_V\rangle}{\langle\Psi^f_V|\Psi^f_V\rangle}} \ ,$$

$$\langle O(\tau)\rangle_{M_f} = \frac{\langle\Psi^f(\tau)|O|\Psi^i_V\rangle}{\langle\Psi^f(\tau)|\Psi^f_V\rangle}\sqrt{\frac{\langle\Psi^f_V|\Psi^f_V\rangle}{\langle\Psi^i_V|\Psi^i_V\rangle}} \ ,$$

Isospin-mixing matrix elements in keV

		H_{01}	K^{CSB}	V^{CSB}	V_γ	(Coul)	(MM)
$2^+;1\Leftrightarrow 2_2^+;0$	GFMC	$-115(3)$	$-3.1(2)$	$-21.3(6)$	$-90.3(26)$	$-78.3(25)$	$-12.0(2)$
	Barker	$-145(3)$				-67	
$1^+;1\Leftrightarrow 1^+;0$	GFMC	$-102(4)$	$-2.9(2)$	$-18.2(6)$	$-80.3(30)$	$-79.5(30)$	$-0.8(2)$
	Barker	$-120(1)$				-54	
$3^+;1\Leftrightarrow 3^+;0$	GFMC	$-90(3)$	$-2.5(2)$	$-14.8(6)$	$-73.1(21)$	$-60.9(21)$	$-12.2(2)$
	Barker	$-62(15)$				-32	
$2^+;1\Leftrightarrow 2_1^+;0$	GFMC	$-6(2)$	$-0.4(2)$	$-1.3(4)$	$-4.4(12)$		

Barker, Nucl.Phys. **83**, 418 (1966)

Coulomb terms are about half of H_{01}, but magnetic moment and strong Type III CSB are relatively more important than in Nolen-Schiffer anomaly; still missing $\approx 20\%$ of strength.

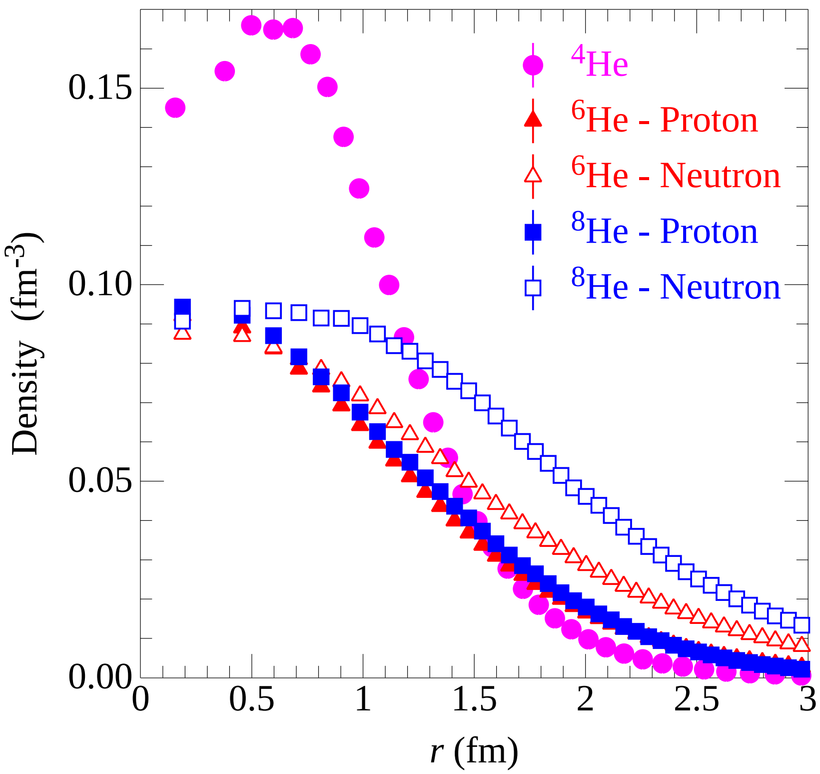
Strong Type IV CSB will also contribute (probably best nuclear structure place to look):

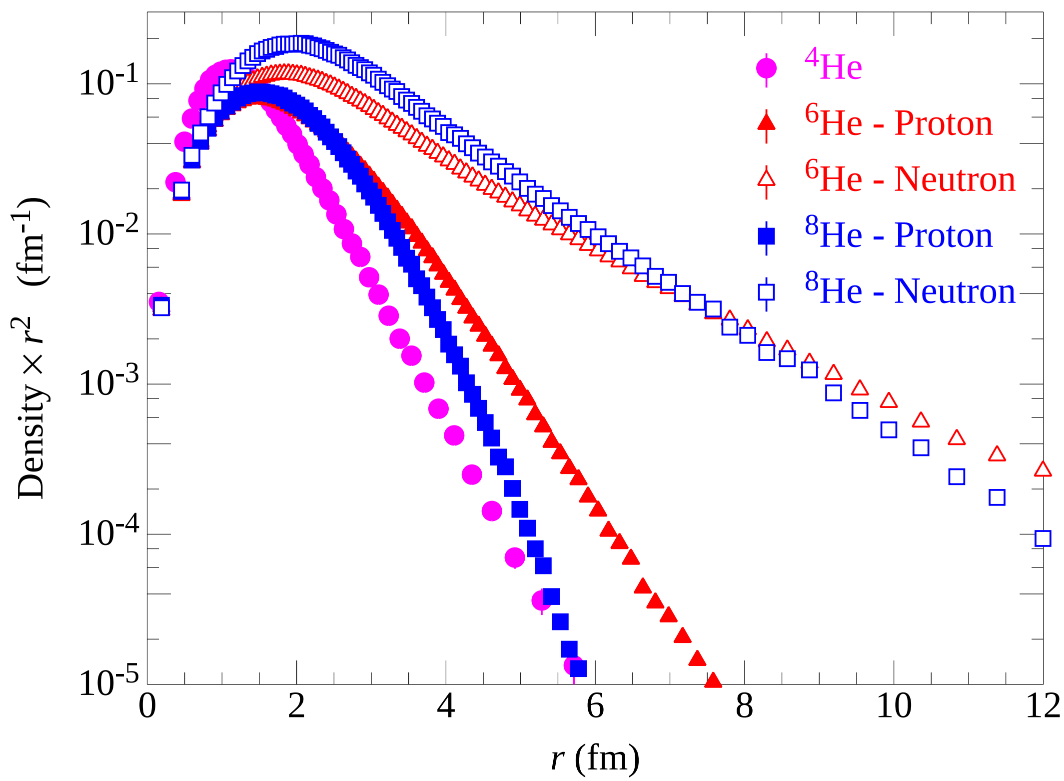
$$V_{IV}^{CSB} = (\tau_1 - \tau_2)_z(\sigma_1 - \sigma_2)\cdot \mathbf{L}\, v(r) + (\tau_1 \times \tau_2)_z(\sigma_1 \times \sigma_2)\cdot \mathbf{L}\, w(r)$$

Preliminary result: $V_{IV}^{CSB} \sim$ few keV.

Single-nucleon densities

$$\rho_{p,n}(r) = \sum_i \langle \Psi | \delta(r - r_i) \frac{1 \pm \tau_i}{2} | \Psi \rangle$$





RMS radii

	r_n	r_p	r_c	Expt
^{4}He	1.45(1)	1.45(1)	1.67(1)	1.681(4)*
^{6}He	2.86(6)	1.92(4)	2.06(4)	2.060(8)†
^{8}He	2.79(3)	1.82(2)	1.94(2)	1.959(16)‡

*Sick, PRC **77**, 041302(R) (2008)

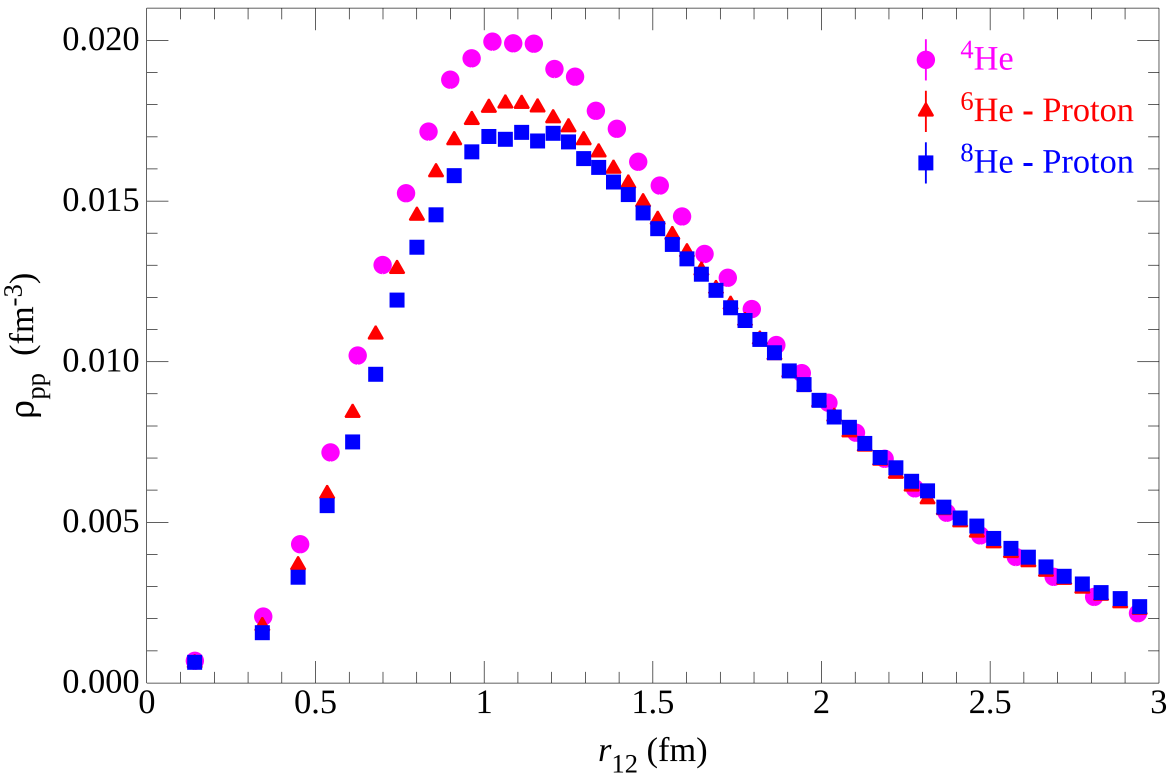
†Wang, *et al.*, PRL **93**, 142501 (2004)

‡Mueller, *et al.*, PRL **99**, 252501 (2007)

Brodeur, *et al.*, PRL **108**, 052504 (2012)

TWO-NUCLEON DENSITIES

$$\rho_{pp}(r) = \sum_{i<j} \langle \Psi | \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \frac{1+\tau_i}{2} \frac{1+\tau_j}{2} | \Psi \rangle$$



RMS radii

	r_{pp}	r_{np}	r_{nn}
^{4}He	2.41	2.35	2.41
^{6}He	2.51	3.69	4.40
^{8}He	2.52	3.58	4.37

INTRINSIC DENSITY OF ^{8}BE

^{8}Be w.f.: ^{4}He core + 4 p-shell nucleons + pair corr.

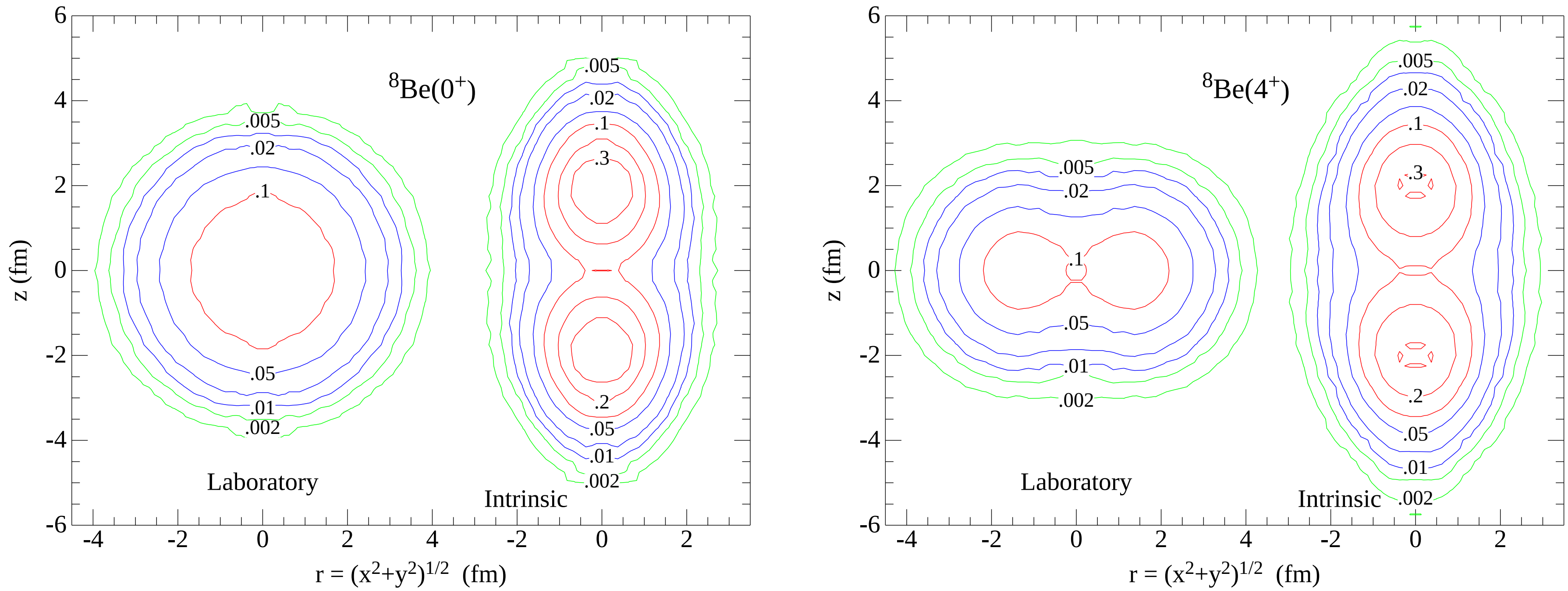
M. C. $\rho(\mathbf{r})$: random walk in $|\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)|^2$ & periodically for each set $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)$

Lab $\rho(\mathbf{r})$: bin $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8$

Intrinsic $\rho(\mathbf{r})$: find eigenvectors of moment of inertia matrix:

$$\mathcal{M} = \sum_i \begin{pmatrix} x_i^2 & x_i y_i & x_i z_i \\ y_i x_i & y_i^2 & y_i z_i \\ z_i x_i & z_i y_i & z_i^2 \end{pmatrix} ,$$

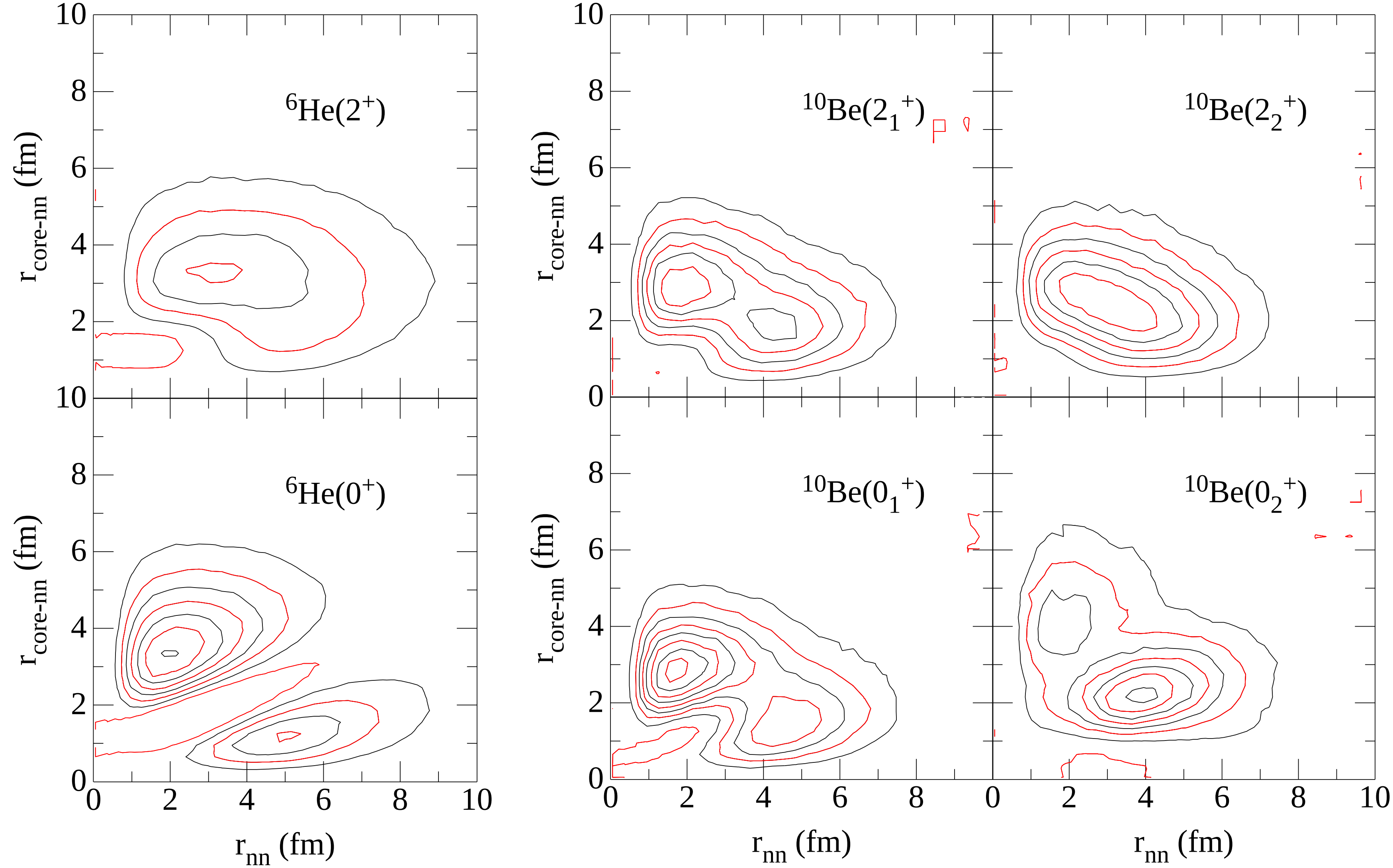
rotate to them, and bin $\mathbf{r}'_1, \mathbf{r}'_2, \cdots, \mathbf{r}'_8$.



Wiringa, Pieper, Carlson, & Pandharipande, Phys. Rev. C **62**, 014001 (2000)

Two-nucleon halo densities

$$\rho_{nn}(r) = \sum_{i<j} \langle \Psi(J^\pi, T, T_z = +1) | \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \tau_i^+ \tau_j^+ | \Psi(J^\pi, T, T_z = -1) \rangle$$

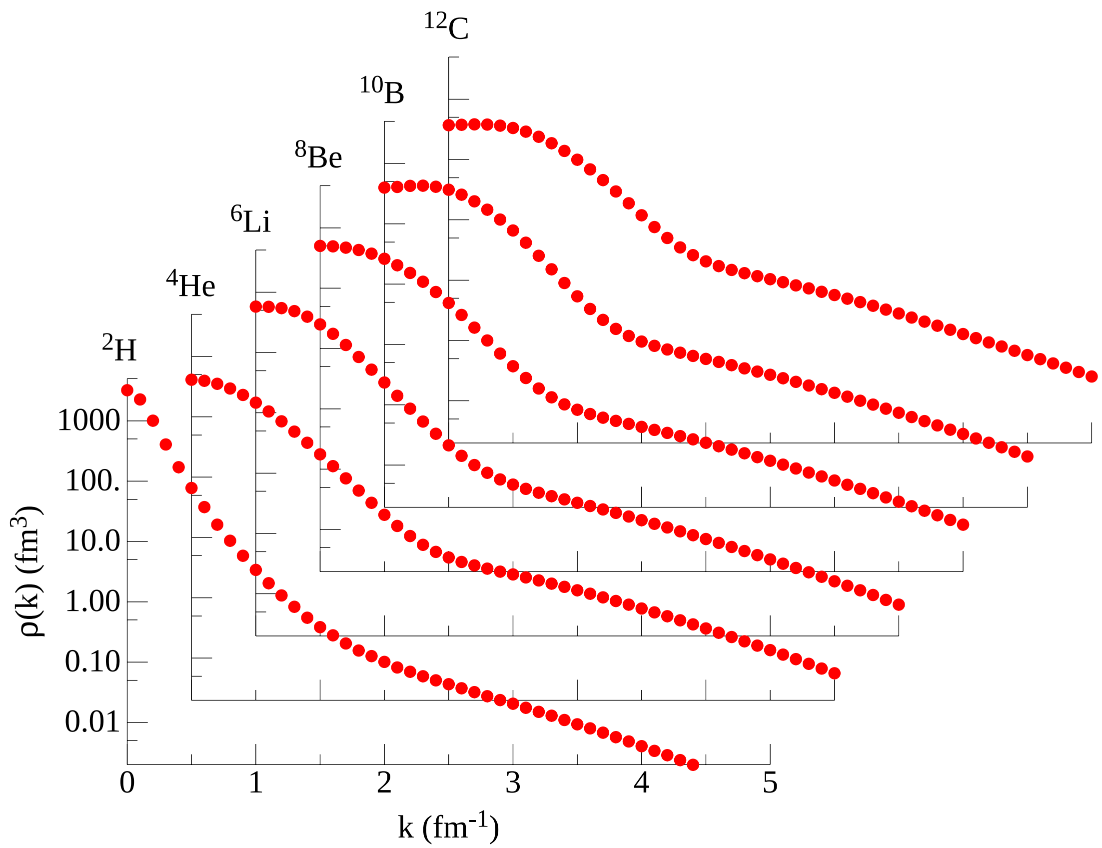


Nucleon momentum distributions

Probability of finding a nucleon in a nucleus with momentum k in a given spin-isospin state:

$$\rho_{\sigma\tau}(k) = \int d\mathbf{r}'_1 d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_A \, \psi^\dagger_A(\mathbf{r}'_1, \mathbf{r}_2, \ldots, \mathbf{r}_A) \, e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1)} \, P_{\sigma\tau} \, \psi_A(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$$

- Useful input for electron scattering studies
- Universal character of high-momentum tails from np tensor interaction



VMC tabulations for $A = 2 - 12$ available at: www.phy.anl.gov/theory/research/momenta

$M1$, $E2$, F, GT transitions

NO EFFECTIVE CHARGES!

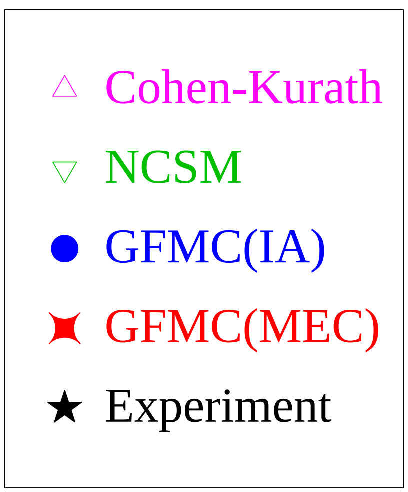
$$E2 = e\sum_k \frac{1}{2}\left[r_k^2 Y_2(\hat{r}_k)\right](1+\tau_{kz})$$

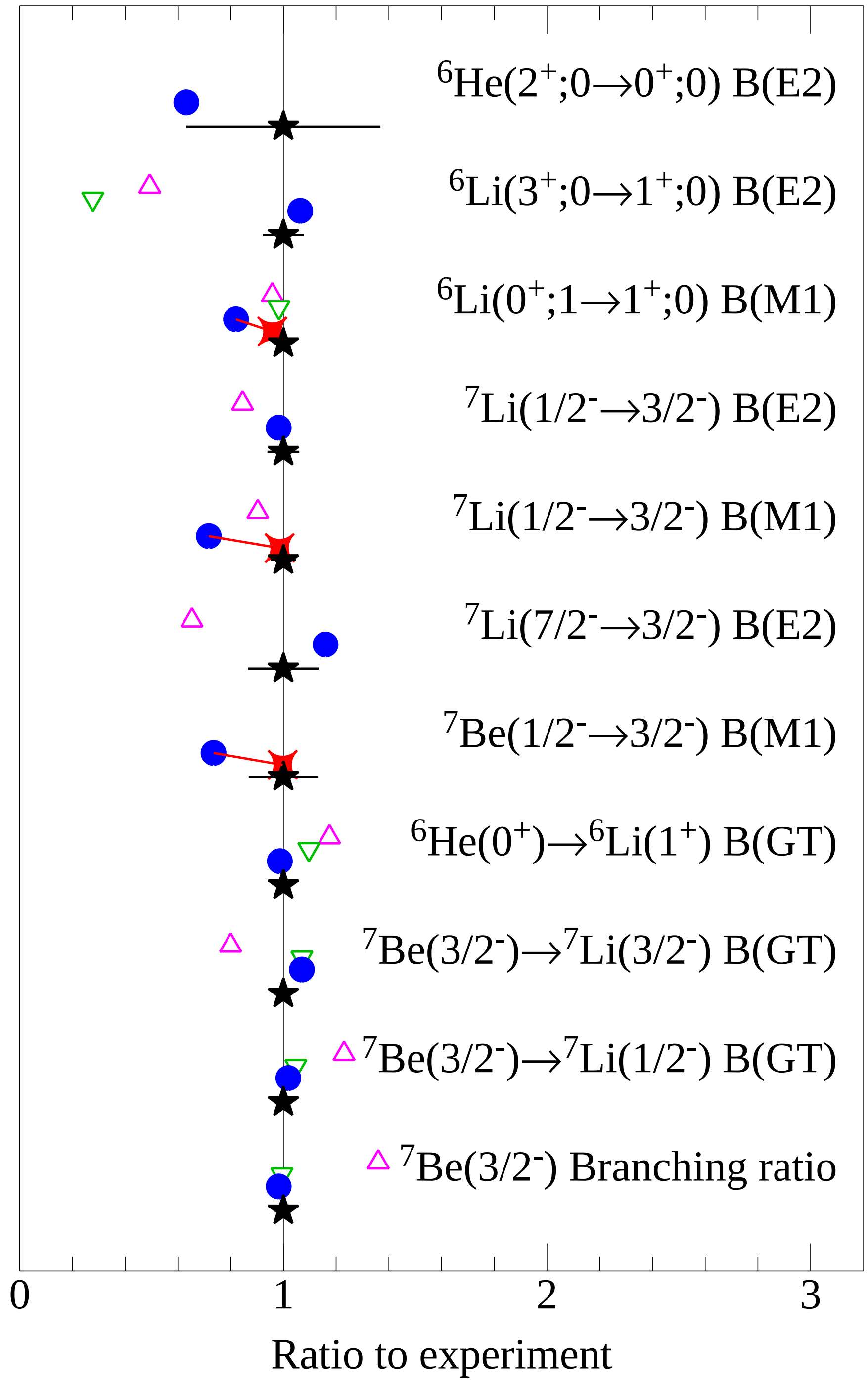
$$M1 = \mu_N \sum_k [(L_k + g_p S_k)(1+\tau_{kz})/2 + g_n S_k \ (1-\tau_{kz})/2]$$

$$\mathrm{F} = \sum_k \tau_{k\pm} \ ; \ \mathrm{GT} = \sum_k \sigma_k \tau_{k\pm}$$

Pervin, Pieper & Wiringa, PRC **76**, 064319 (2007)

Marcucci, Pervin, *et al.*, PRC **78**, 065501 (2008)

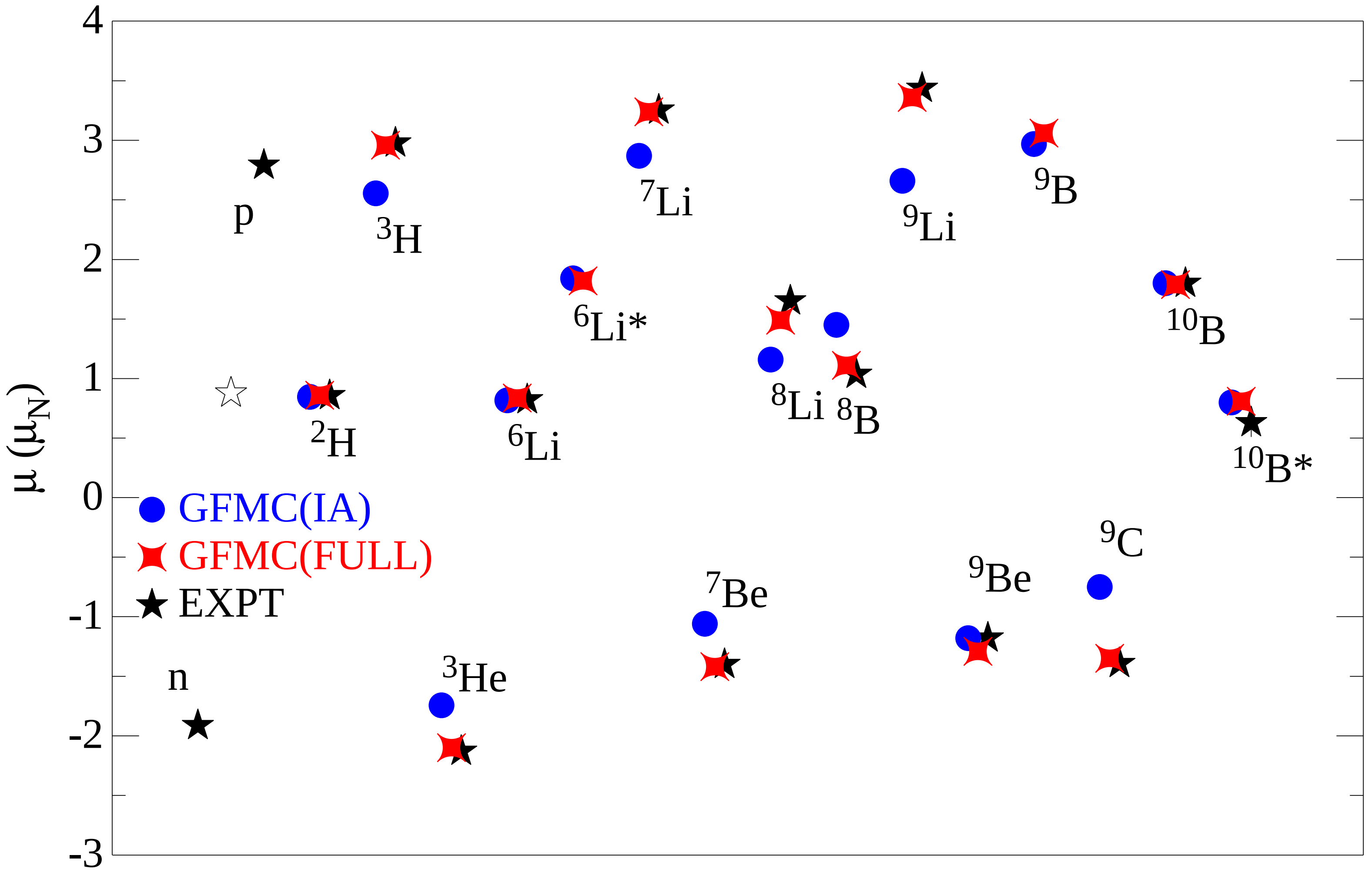




$A \leq 10$ Magnetic moments w/ χEFT exchange currents

Hybrid calculations using AV18+IL7 wave functions and χEFT exchange currents developed in:

Pastore, Schiavilla, & Goity, PRC **78**, 064002 (2008) ; Pastore, *et al.*, PRC **80**, 034004 (2009)

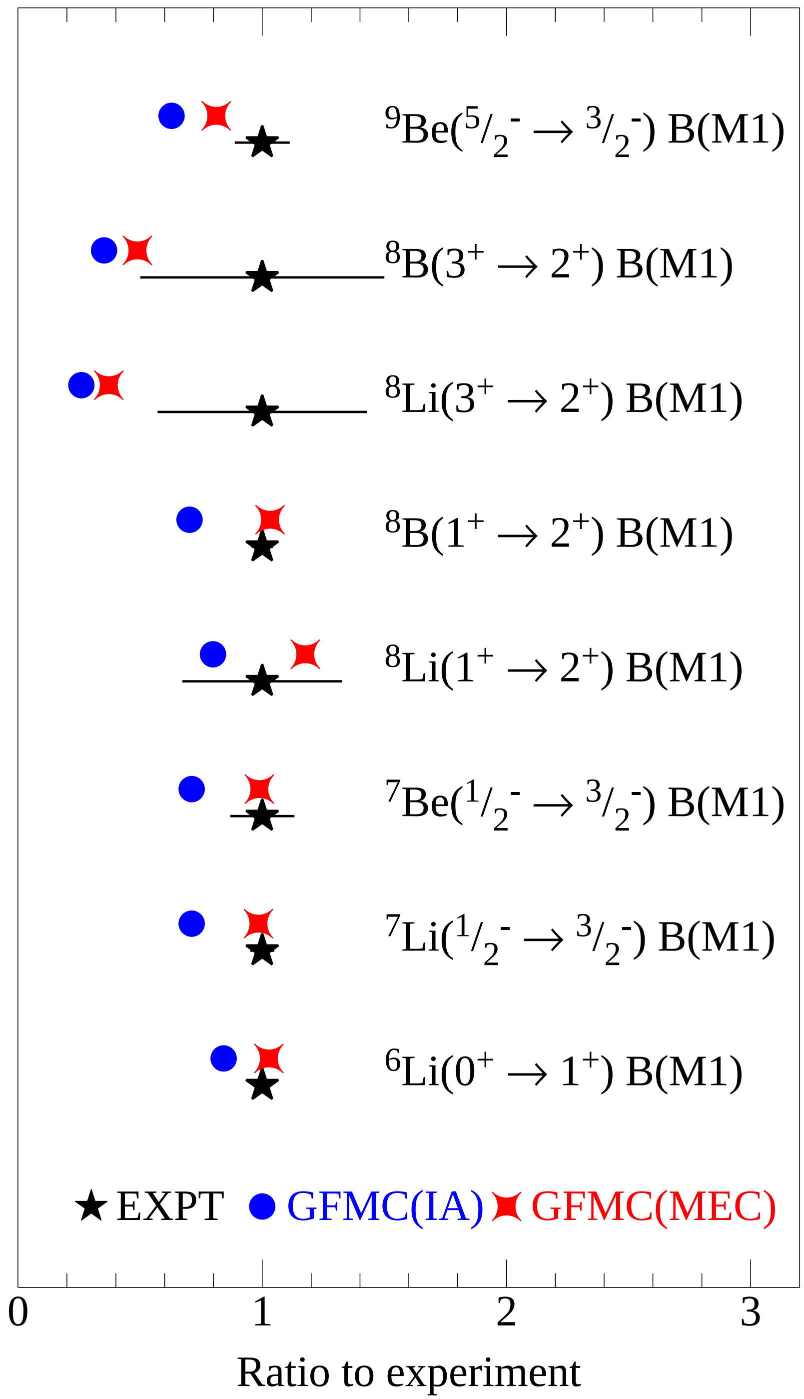


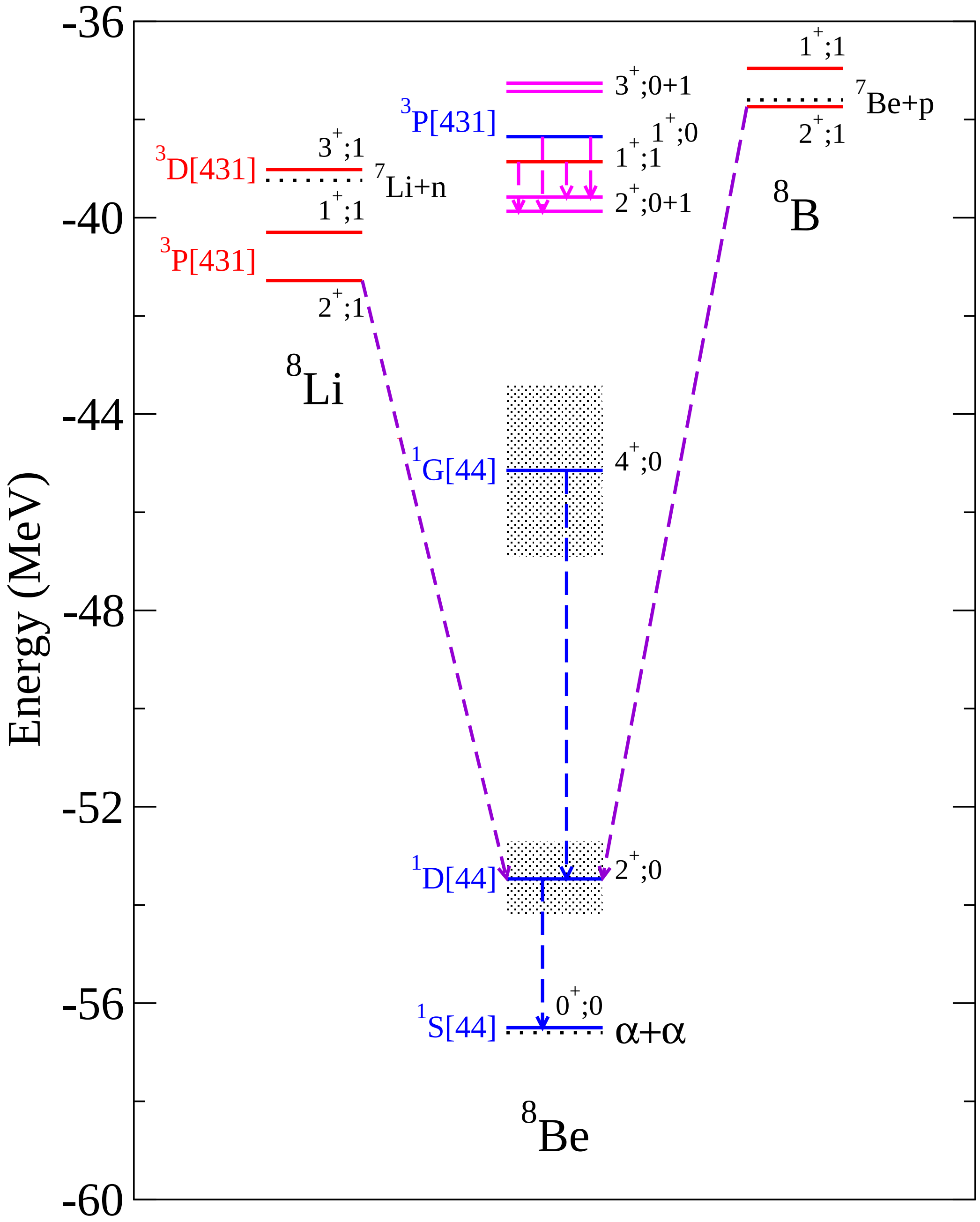
$M1$ TRANSITIONS W/ χEFT

- dominant contribution is from OPE
- five LECs at N3LO
- d_2^V and d_1^V are fixed assuming Δ resonance saturation
- d^S and c^S are fit to experimental μ_d and $\mu_S(^3\text{H}/^3\text{He})$
- c^V is fit to experimental $\mu_V(^3\text{H}/^3\text{He})$
- $\Lambda = 600$ MeV

Pastore, Pieper, Schiavilla & Wiringa

PRC **87**, 035503 (2013)





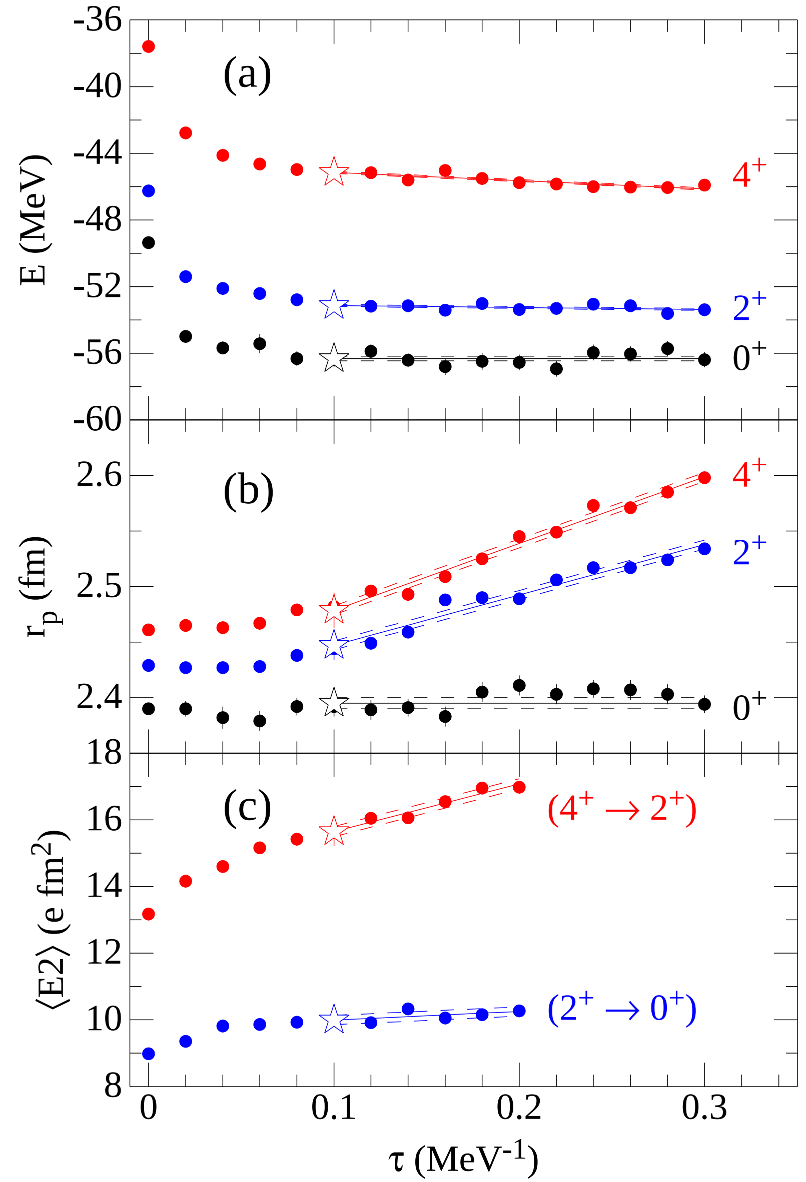
Transitions in/to ^{8}Be

- ^{8}Be presents new challenges in transition calculations
- $E2$ transitions between rotational band states which have large widths
- $M1$ transitions involving isospin-mixed states
- GT transitions that are not super-allowed and go to a broad final state

$J^\pi; T$	GFMC	Expt
0^+	-56.3(2)	-56.50
2^+	+ 3.2(2)	+ 3.03(1)
4^+	+11.2(2)	+11.35(15)
$2^+; 0$	+16.8(3)	+16.746(3) $\longrightarrow$ 16.626
$2^+; 1$	+16.8(3)	+16.802(3) $\longrightarrow$ 16.922
$1^+; 1$	+17.4(2)	+17.67 $\longrightarrow$ 17.64
$1^+; 0$	+18.0(3)	+18.12 $\longrightarrow$ 18.15

$E2$ TRANSITIONS IN ^{8}Be

- New experiment at Tata Institute, Mumbai for $4^+ \rightarrow 2^+$ transition
- Experimental AND theoretical challenge: 4^+ and 2^+ states are wide and breakup into two αs
- GFMC calculation is extrapolated back to $\tau = 0.1$ MeV^{-1}; predicts $B(E2)$ = 27.2(15)
- Experiment detects α+α+γ in coincidence for range of beam energies
- Assuming Breit-Wigner shape, simple analysis gives $B(E2)$ = 21.3(23)



Datar, Chakrabarty, Kumar, Nanal, Pastore, Wiringa, et al., arXiv:1305.1094

$M1$ TRANSITIONS IN ^{8}Be BETWEEN ISOSPIN-MIXED STATES

We calculate between states of pure isospin:

matrix element	IA	MEC	TOT
$\langle 1^+;1\vert M1\vert 2^+;0\rangle$	2.29(1)	0.62(1)	2.91(1)
$\langle 1^+;1\vert M1\vert 2^+;1\rangle$	0.14(0)	0.04(1)	0.18(1)
$\langle 1^+;0\vert M1\vert 2^+;0\rangle$	0.17(0)	0.02(0)	0.19(0)
$\langle 1^+;0\vert M1\vert 2^+;1\rangle$	2.60(1)	0.29(1)	2.89(1)

Then have to combine them using the physical states:

$$|16.626\rangle = 0.77|2^+;0\rangle + 0.64|2^+;1\rangle \qquad |17.64\rangle = 0.24|1^+;0\rangle + 0.97|1^+;1\rangle$$

$$|16.922\rangle = 0.64|2^+;0\rangle - 0.77|2^+;1\rangle \qquad |18.15\rangle = 0.97|1^+;0\rangle - 0.24|1^+;1\rangle$$

to get the final results:

$B(M1)$	IA	TOT	Expt
17.64 $\longrightarrow$ 16.626	1.65(2)	2.54(3)	2.65(25)
17.64 $\longrightarrow$ 16.922	0.25(1)	0.46(1)	0.30(7)
18.15 $\longrightarrow$ 16.626	0.56(1)	0.62(1)	1.88(46)
18.15 $\longrightarrow$ 16.922	1.56(2)	2.01(2)	2.89(33)

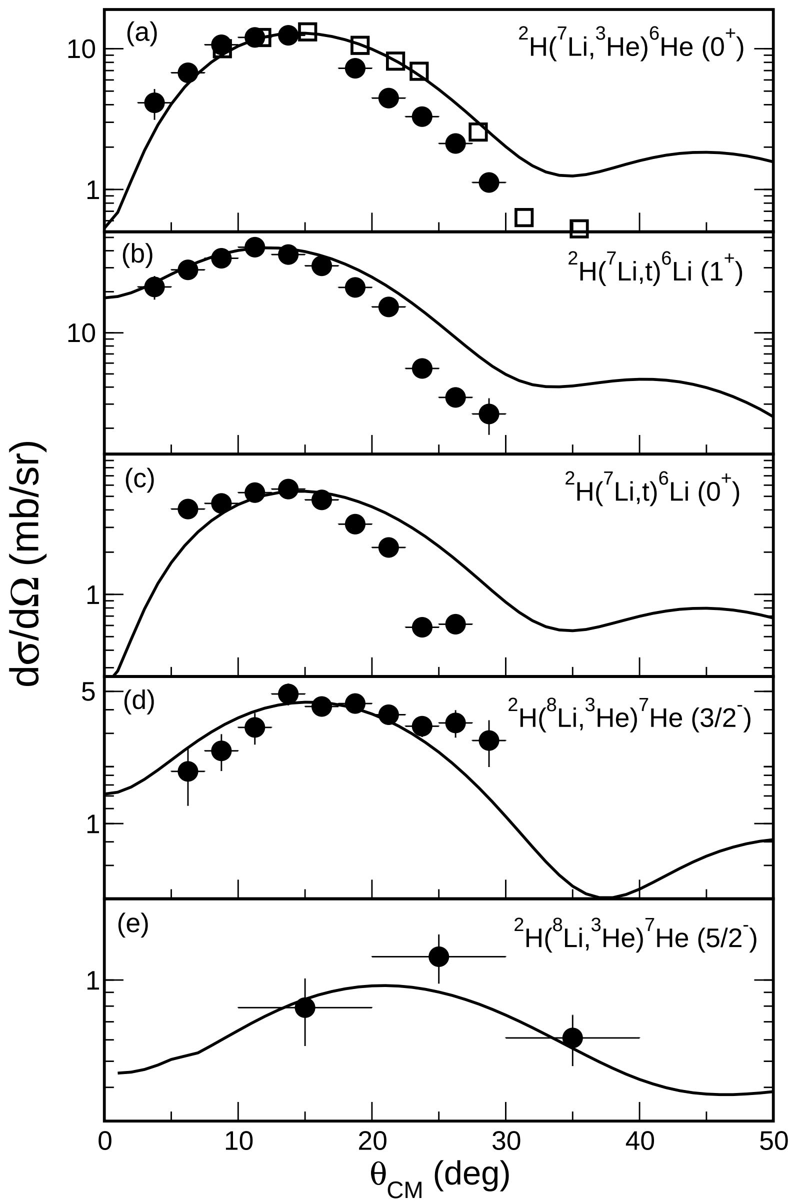
We evaluate the isospin-mixing matrix elements $\langle H_{01}\rangle$ to make sure we have the correct relative signs of our wave functions.

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), $(^{8}\text{Li},^{9}\text{Li})$, etc. vertices computed as A-body overlaps using VMC $\langle\Psi_V(A\text{-}1)|a|\Psi_V(A)\rangle$
- Norm is spectroscopic factor
- Absolute prediction for $d\sigma/d\Omega$
- Good predictions of n-knockout from ^{10}Be and ^{10}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 $\alpha \equiv [J^\pi_A, T_A, T_{z_A}]$, $\gamma \equiv [J^\pi_{A-1}, T_{A-1}, T_{z_{A-1}}]$, 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:

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

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

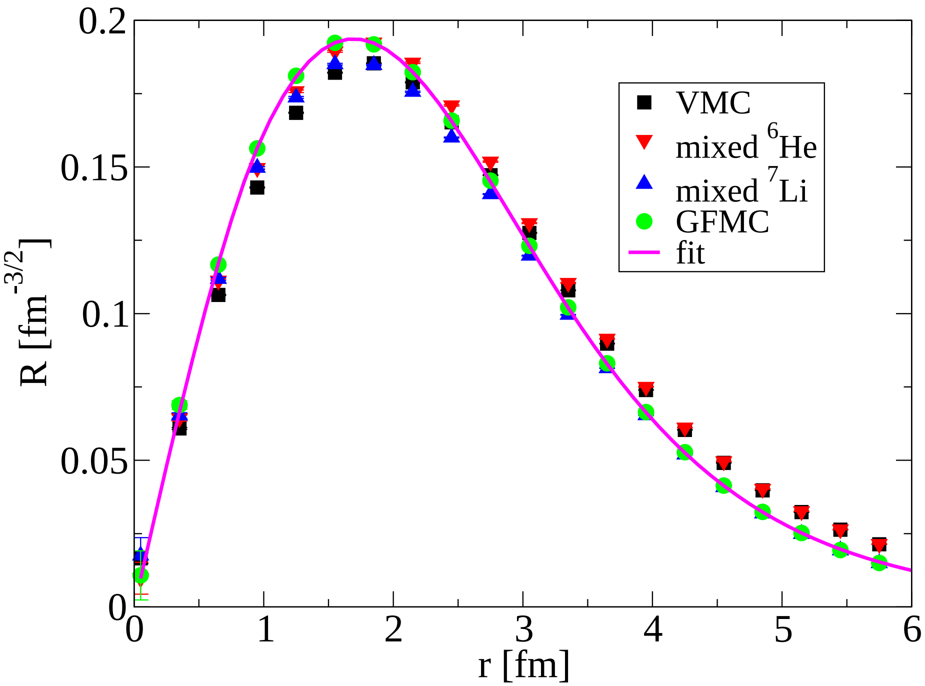
$$R(\alpha,\gamma,\nu;r) \xrightarrow{r\rightarrow\infty} C(\alpha,\gamma,\nu)\frac{W_{-\eta,l+1/2}(2kr)}{r},$$

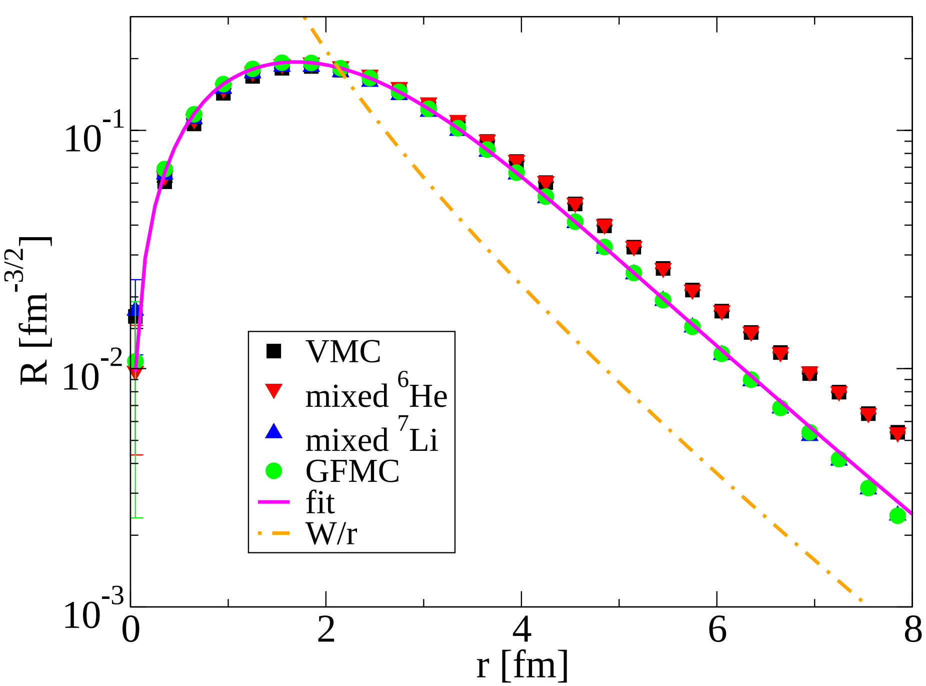
where $W_{-\eta,l+1/2}(2kr)$ is a Whitakker function with $k = \sqrt{2\mu B}/\hbar$, B is the separation energy, and $C(\alpha,\gamma,\nu)$ is the asymptotic normalization coefficient or ANC.

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 $\langle {}^6\mathrm{He} + p\,|{}^7\mathrm{Li}\rangle$

Brida, Pieper, & Wiringa, PRC **84**, 024319 (2011)

GFMC FOR SCATTERING STATES

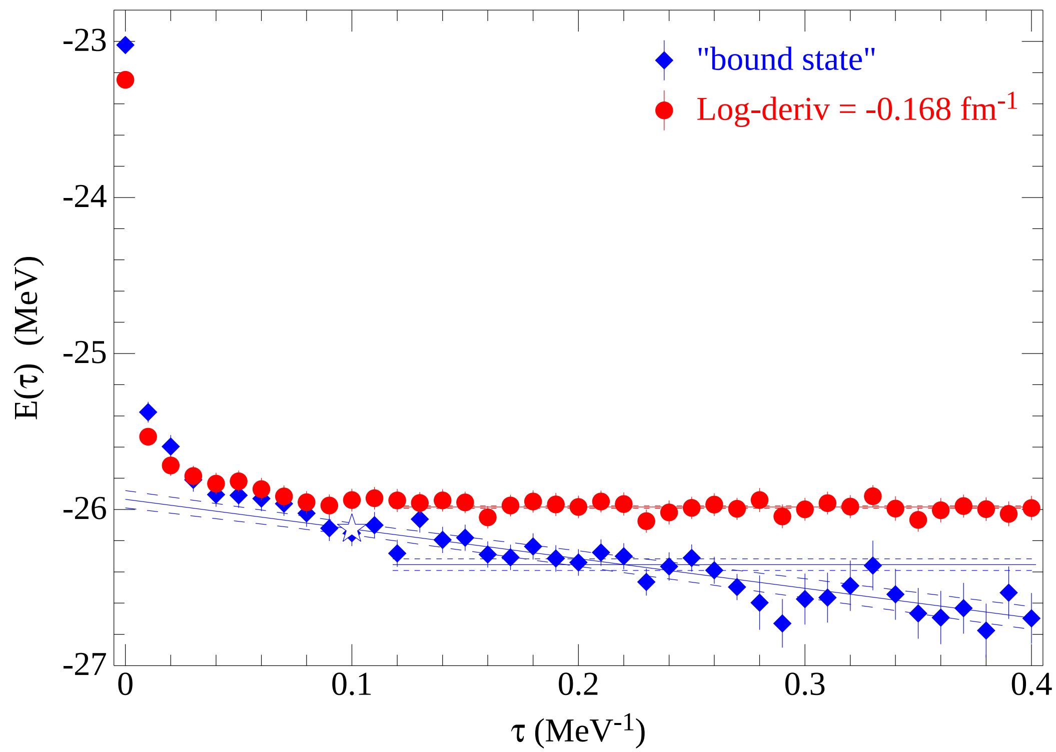
GFMC treats nuclei as particle-stable system – should be good for energies of narrow resonances
Need better treatment for locations and widths of wide states and for capture reactions

METHOD

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

Example for ^{5}He($\frac{1}{2}^-$)

- "Bound-state" boundary condition does not give stable energy; Decaying to n+^{4}He threshold
- Scattering boundary condition produces stable energy.



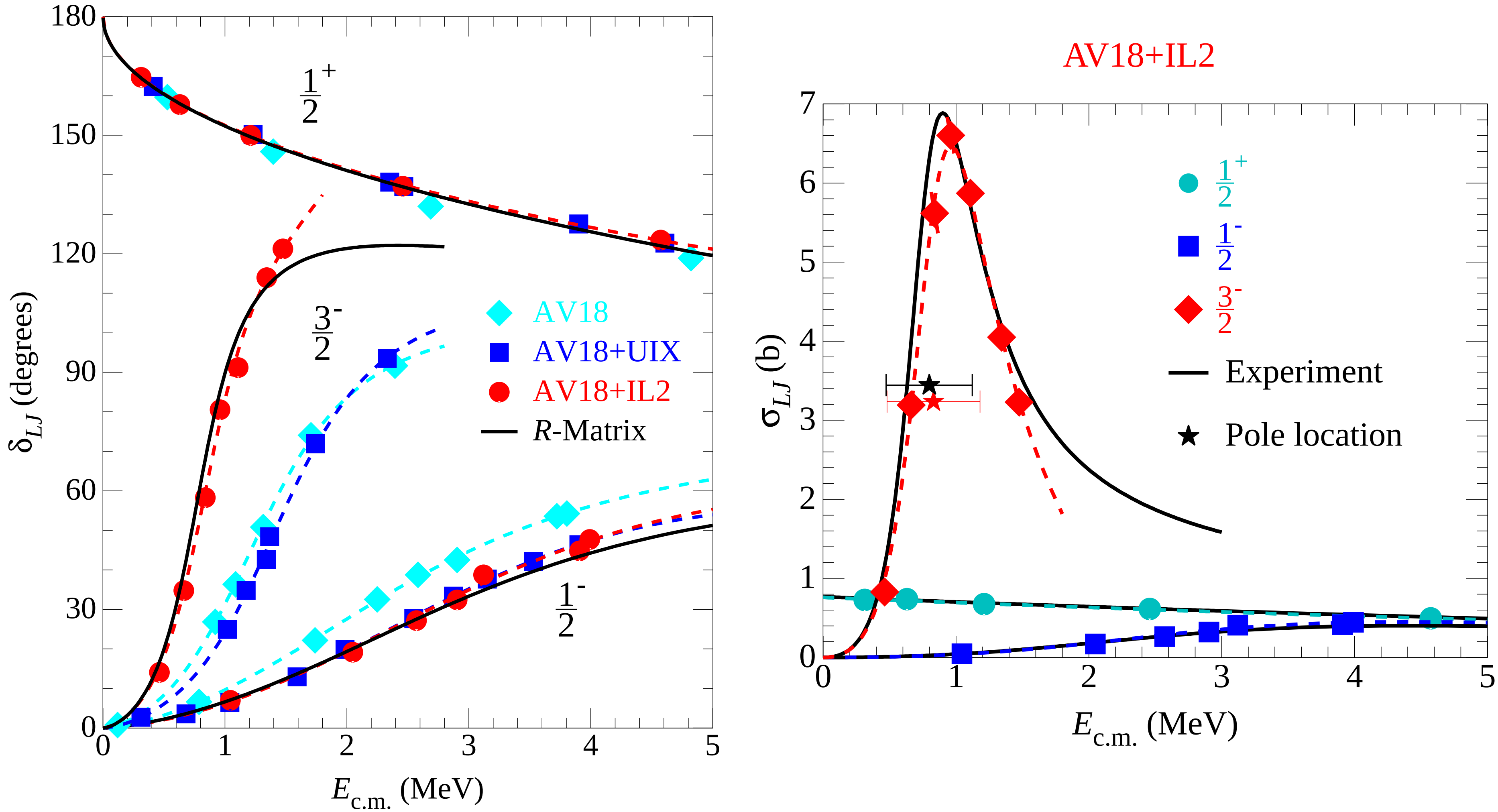
^{5}He AS n+^{4}He SCATTERING

Black curves: Hale phase shifts from R-matrix analysis up to $J = \frac{9}{2}$ of data

AV18 with no V_{ijk} underbinds ^{5}He($3/2^-$) & overbinds ^{5}He($1/2^-$)

AV18+UIX improves ^{5}He($1/2^-$) 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)

Conclusions

We have demonstrated that realistic nuclear Hamiltonians and accurate QMC calculations can reproduce many properties of light nuclei:

- Argonne v_{ij} + Illinois V_{ijk} gives rms binding-energy errors < 0.6 MeV for A = 3–12
- Successfully predict/reproduce densities, radii, moments, & transition matrix elements
- Can obtain energies and widths of low-energy nucleon-nucleus scattering states

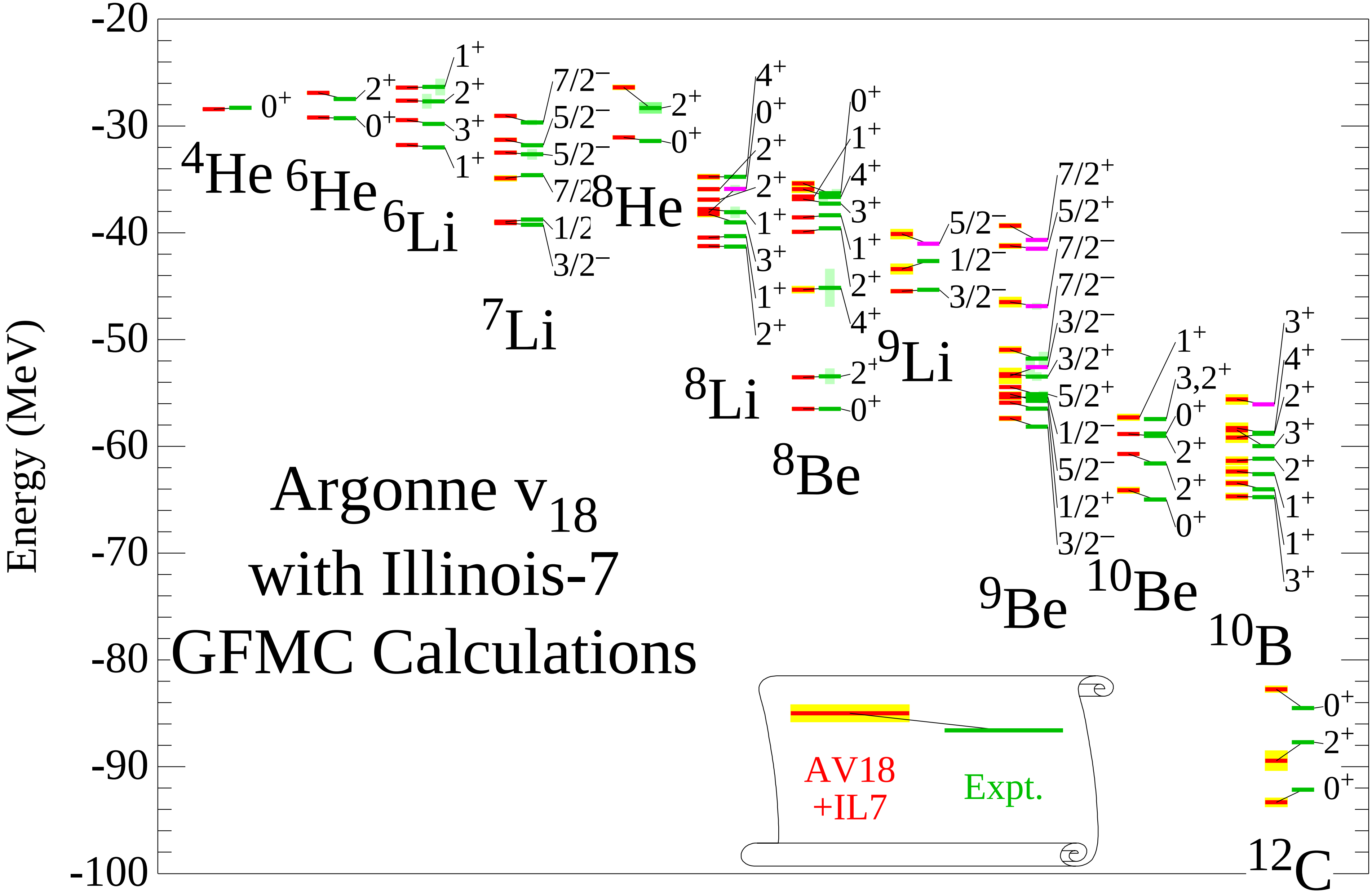
There are many more exciting challenges in the structure and reactions of $A \leq 12$ nuclei, which we want to tackle in the next few years, such as:

- ^{12}C excited states and transitions; ν-^{12}C scattering
- Single- & double-intruder states in ^{9,10,11}Be, ^{10,11}B; ^{11}Li
- More electroweak transitions in $A \leq 12$
- Charge-independence breaking in ^{10}C(β^+)^{10}B
- Parity-violating n-α scattering: $\langle ^5\mathrm{He}(\frac{1}{2}^-)|H_{PV}|^5\mathrm{He}(\frac{1}{2}^+)\rangle$
- Cluster-cluster overlaps, SFs, ANCs, for $\langle (A\text{-}2)d|A\rangle$, $\langle (A\text{-}4)\alpha|A\rangle$
- Astrophysical reactions such as ^{3}He(α,γ)^{7}Be

For larger nuclei $A > 12$ some possibilities are:

- exascale computing for ^{16}O ($\sim 1000\times$ more expensive than ^{12}C)
- cluster GFMC (cluster VMC for ^{16}O done in 1990s)
- AFDMC (auxiliary field diffusion Monte Carlo) or hybrid GFMC-AFDMC

Gandolfi, Pederiva, Fantoni, & Schmidt ('79), PRL **99**, 022507 (2007)



Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
Argonne v18
with Illinois-7
GFMC Calculations
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C
AV18
+IL7
Expt.