The Structure of Light Nuclei

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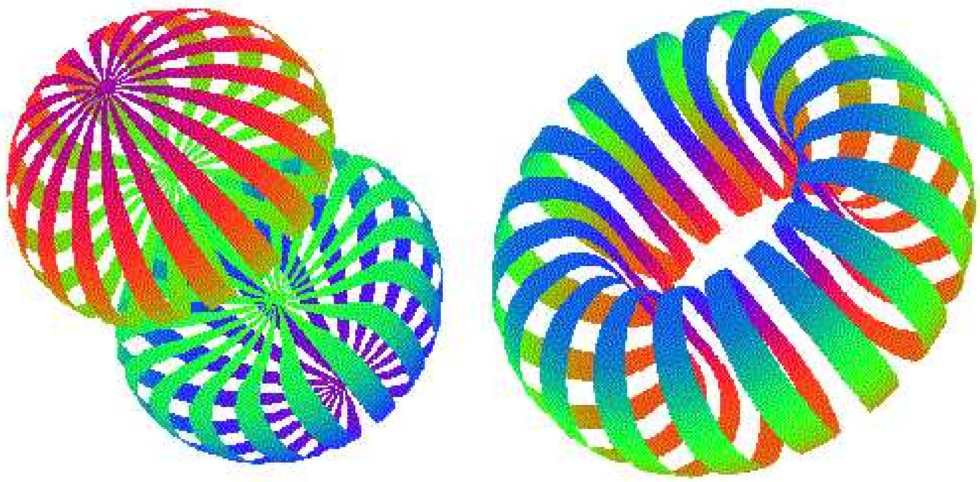

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Physics Division

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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, spectroscopic overlaps
- Low-energy NA & AA' scattering, asymptotic normalizations, electroweak response

Requirements

- Two-nucleon potentials that accurately describe elastic NN scattering data
- Consistent three-nucleon potentials and two-nucleon 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, Coulomb sum calculated
- ^{5}He = $n\alpha$ scattering and $3 \leq A \leq 9$ ANCs and widths

Nuclear Hamiltonian

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

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

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

Argonne v_{18}

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

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

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

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

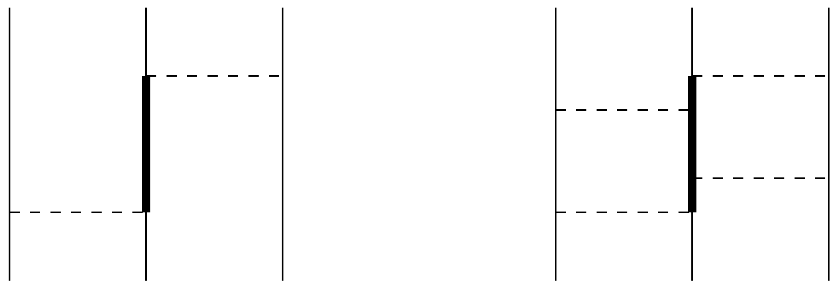
$$v_{ij}^{S} = \sum_p [P^p + Q^p r + R^p r^2]W(r)O_{ij}^p$$

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

Argonne v_{18} fitted to 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

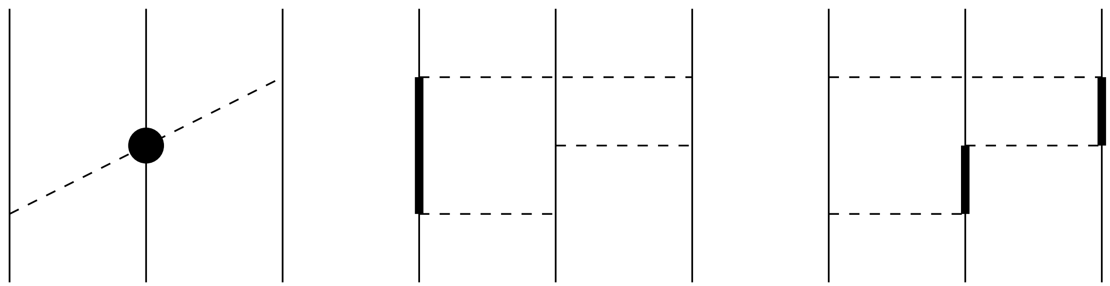
THREE-NUCLEON POTENTIALS

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



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

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



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 Metropolis 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)

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 diffusion 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

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

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

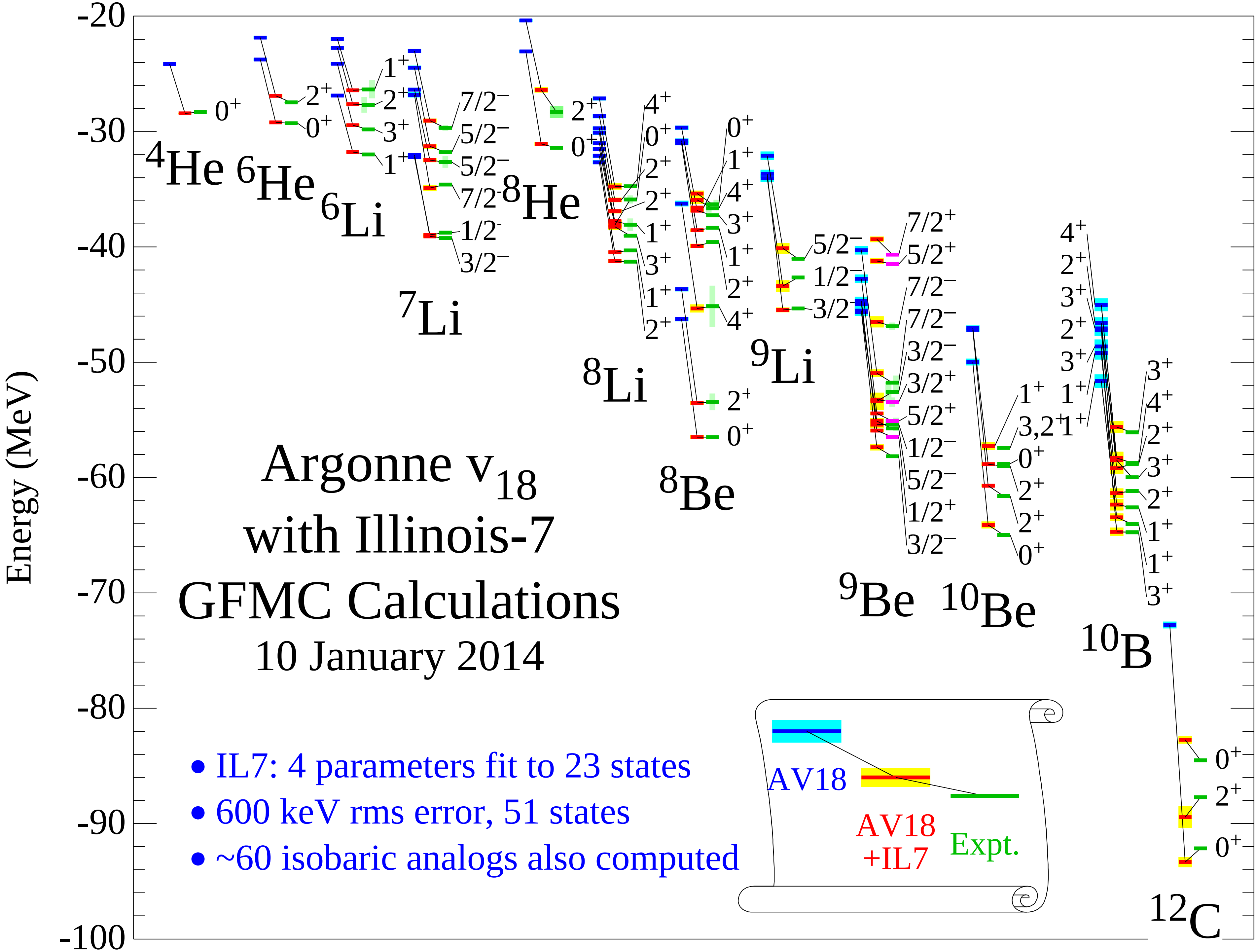
- Cannot propagate p^2, L^2, or $(\mathbf{L}\cdot\mathbf{S})^2$ operators ⇒ use H' = AV8′ + $\tilde{V}_{ijk}$
- Fermion sign problem would limit maximum τ, but ...
- Constrained-path propagation removes steps that have $\overline{\Psi^\dagger(\tau,\mathbf{R})\Psi_V(\mathbf{R})} = 0$
- Multiple excited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

Carlson, PRC **38**, 1879 (1988)

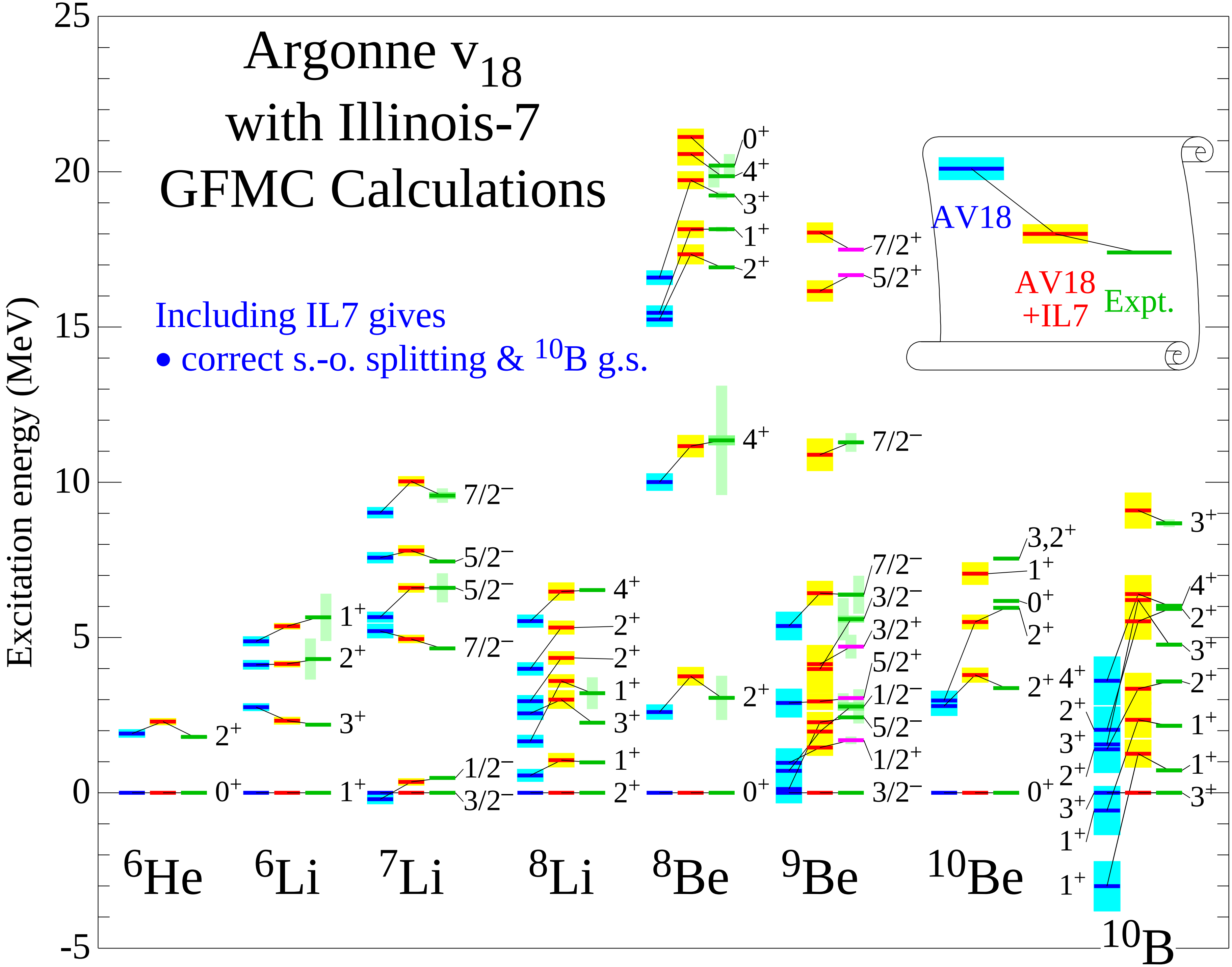
Pudliner, Pandharipande, Carlson, Pieper, & Wiringa, PRC **56**, 1720 (1997)

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

Pieper, Wiringa, & Carlson, PRC **70**, 054325 (2004)



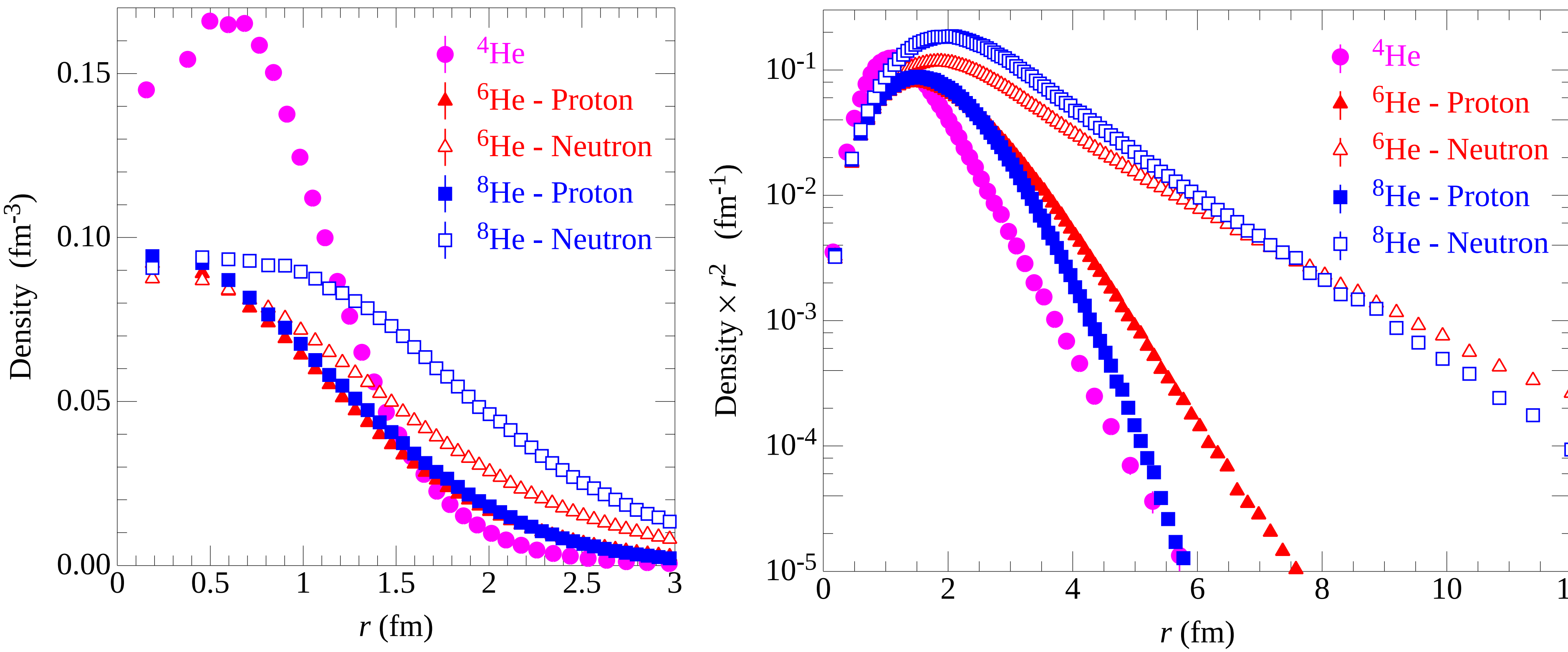
Energy (MeV)
Argonne v18
with Illinois-7
GFMC Calculations
10 January 2014
• IL7: 4 parameters fit to 23 states
• 600 keV rms error, 51 states
• ~60 isobaric analogs also computed
AV18
AV18
+IL7
Expt.
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C



Argonne v_{18}
with Illinois-7
GFMC Calculations
Including IL7 gives
• correct s.-o. splitting & ^{10}B g.s.
AV18
AV18 +IL7
Expt.
Excitation energy (MeV)
25
20
15
10
5
0
-5
^{6}He
^{6}Li
^{7}Li
^{8}Li
^{8}Be
^{9}Be
^{10}Be
^{10}B

SINGLE-NUCLEON DENSITIES

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



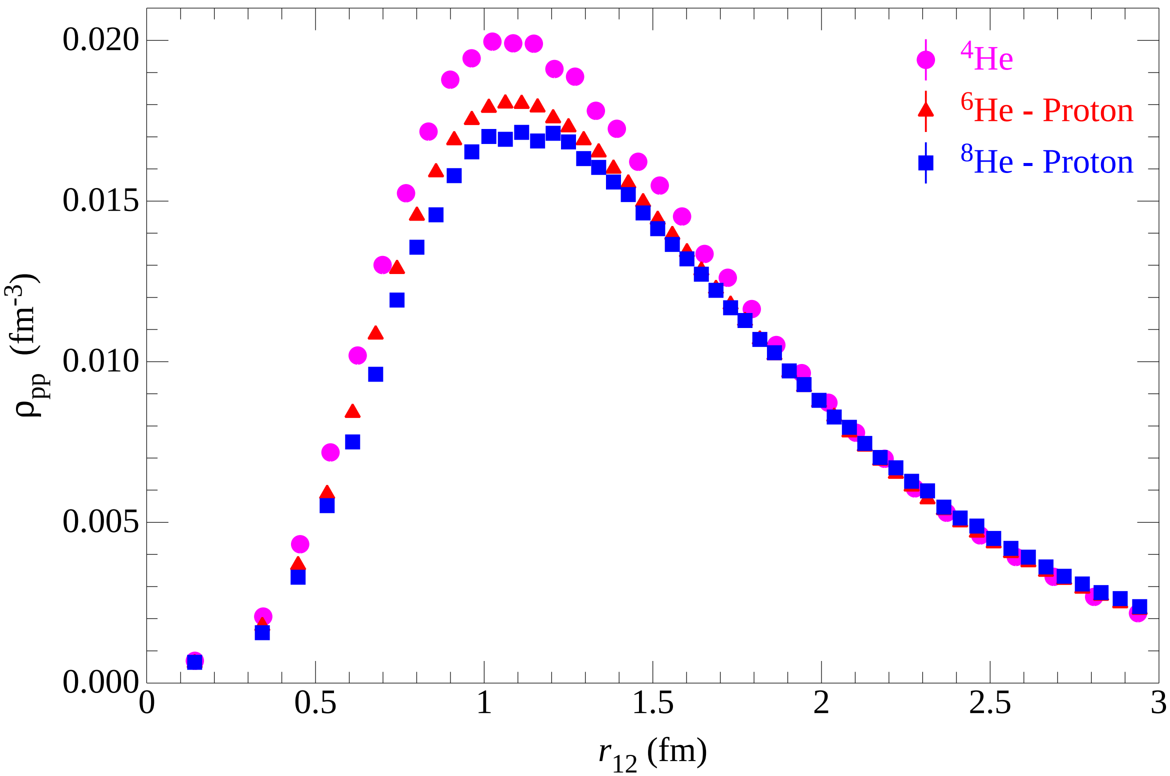
RMS radii

	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

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

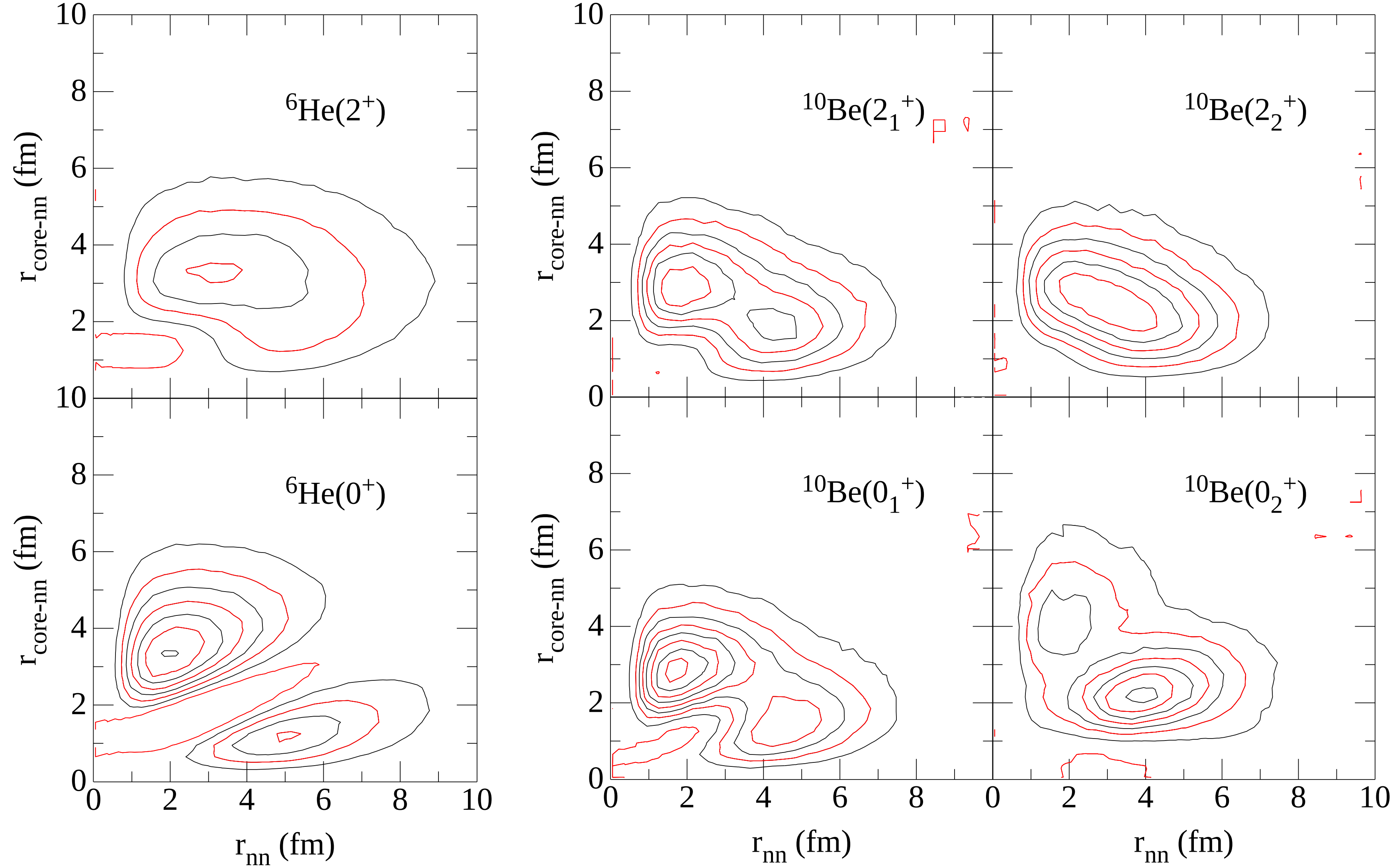


RMS radii

	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

Two-nucleon halo densities

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



INTRINSIC DENSITY OF ^{8}BE

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

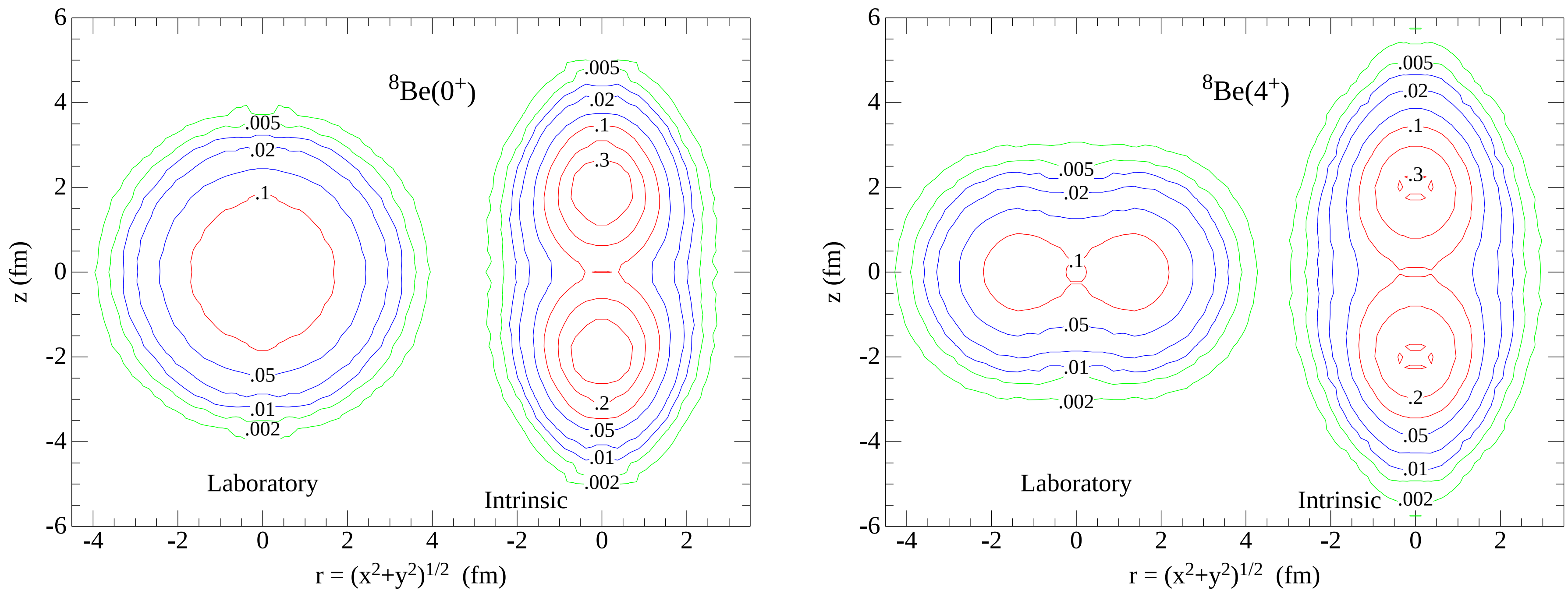
M. C. $\rho(\mathbf{r})$: random walk in $|\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)|^2$ & periodically for each set $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_8)$

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 $\mathbf{r}'_1, \mathbf{r}'_2, \cdots, \mathbf{r}'_8$.

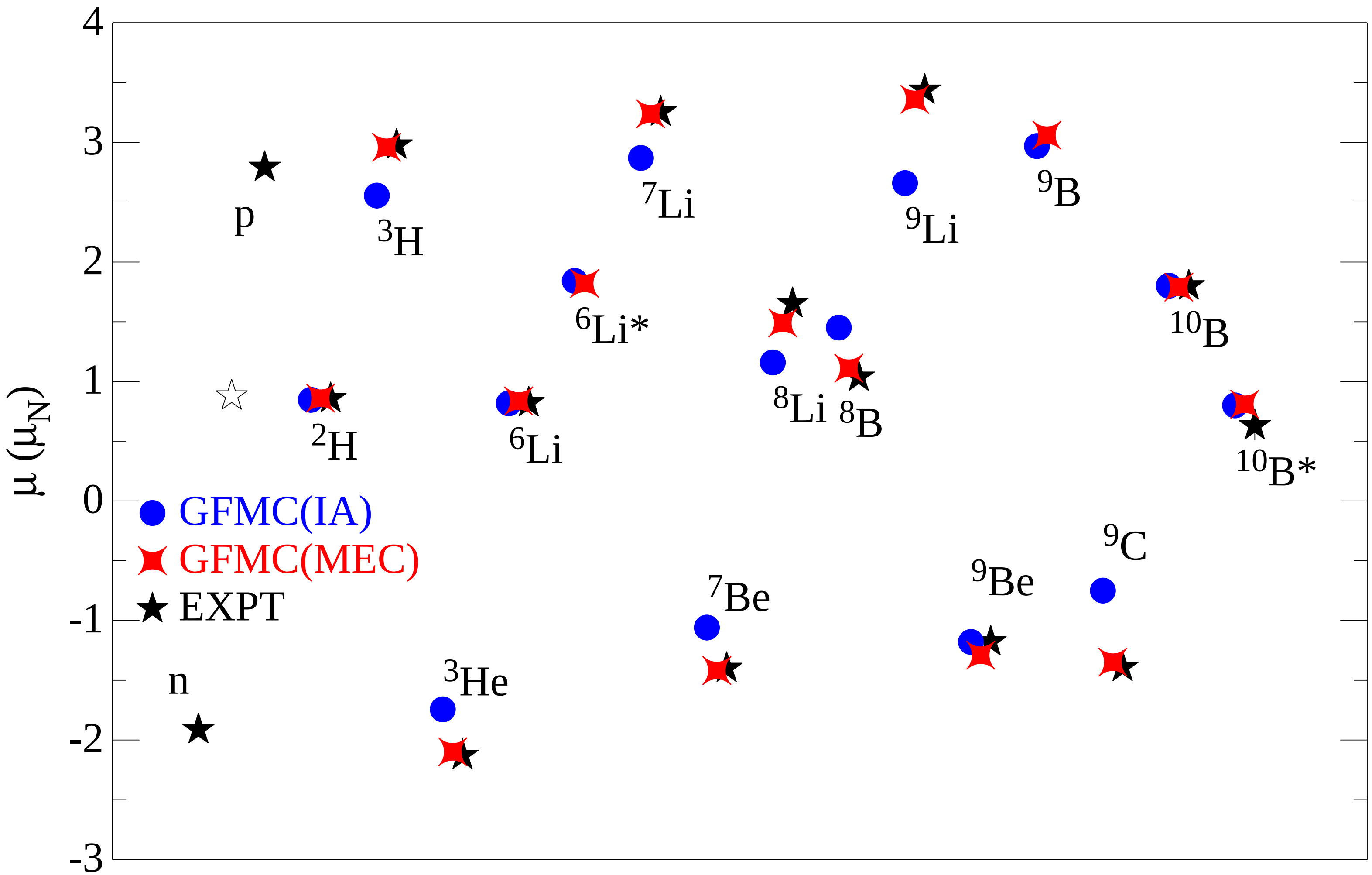


Wiringa, Pieper, Carlson, & Pandharipande, Phys. Rev. C **62**, 014001 (2000)

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

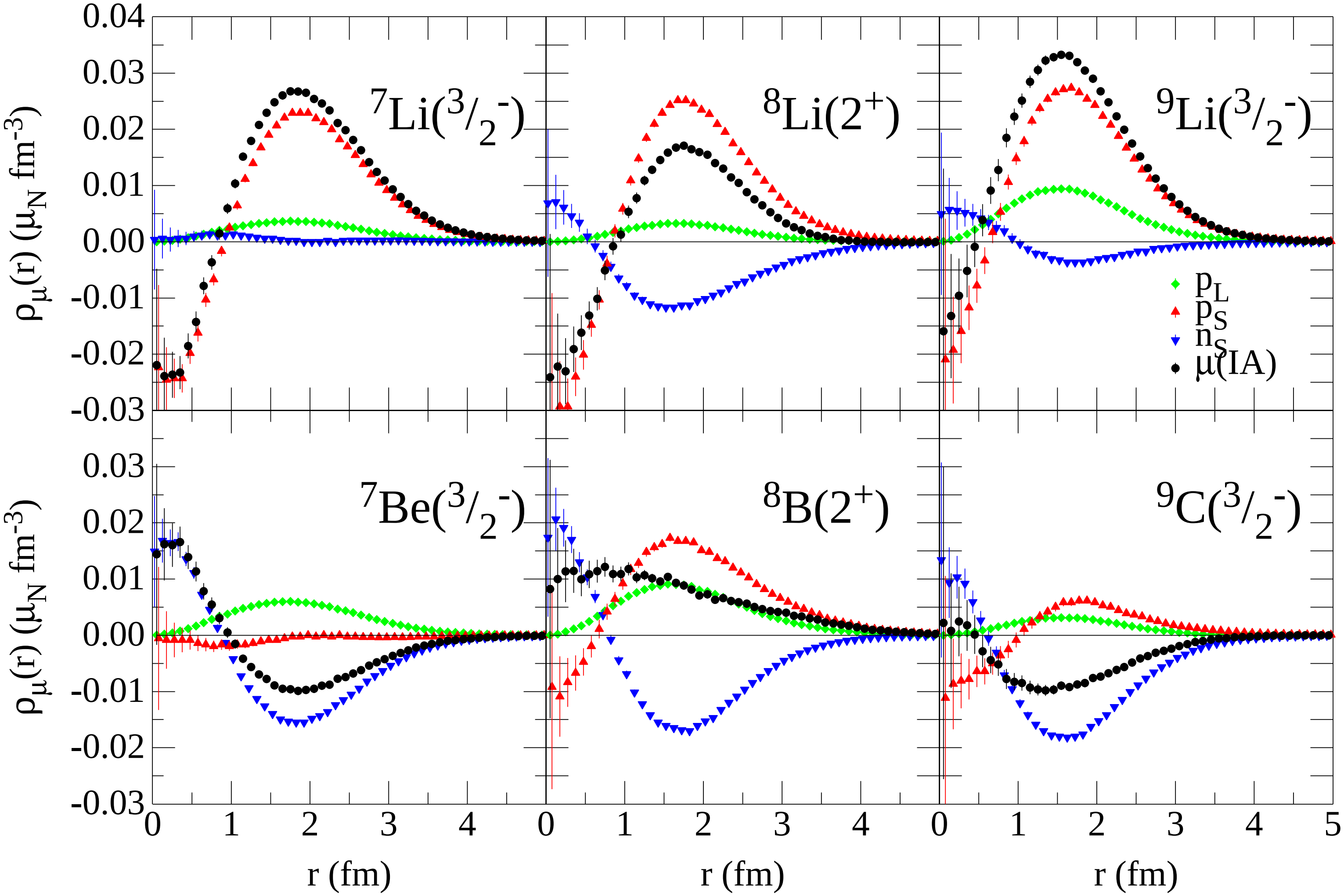
Hybrid calculations using AV18+IL7 wave functions and χEFT exchange currents developed in:

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



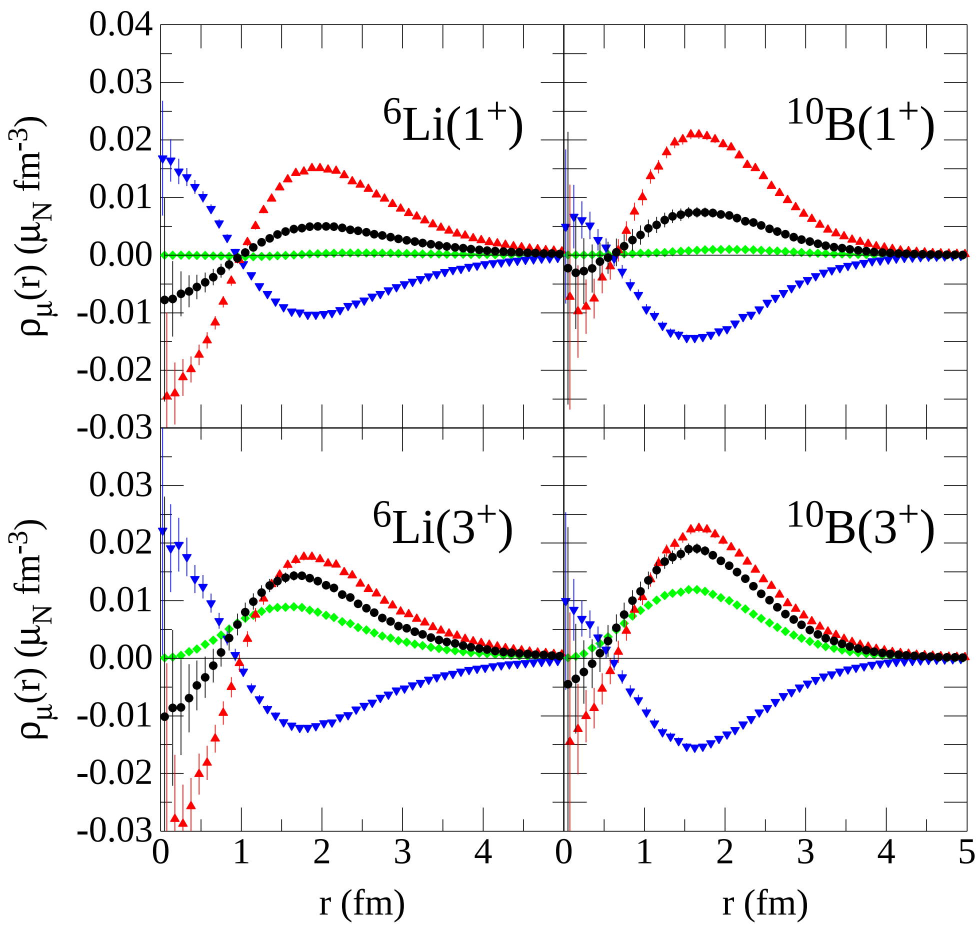
Pastore, Pieper, Schiavilla & Wiringa, PRC **87**, 035503 (2013)

Magnetic densities



$$\mu_p[\rho_{p\uparrow}(r) - \rho_{p\downarrow}(r)] \quad \mu_n[\rho_{n\uparrow}(r) - \rho_{n\downarrow}(r)] \quad \mu_p \rho_{p\mathbf{L}}(r)$$

Magnetic densities



Magnetic radii

^AZ	VMC	Expt
p		0.777(16)
n		0.862(9)
^{2}H	2.09	1.90(14)
^{3}H	1.85	1.84(18)
^{3}He	1.92	1.965(153)
^{6}Li	3.41	
^{7}Li	2.85	2.98(5)
^{9}Be	3.10	3.2(3)
^{10}B	2.72	

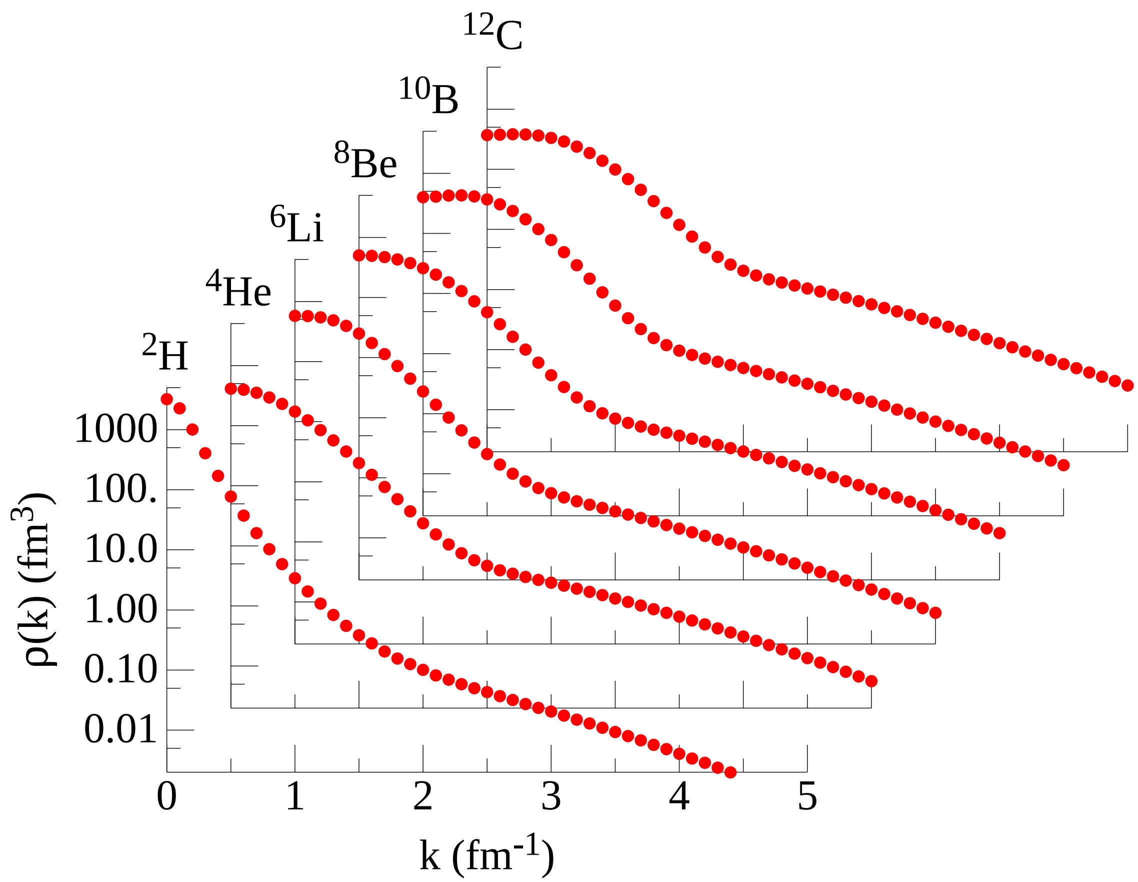
Can these be measured better?

SINGLE-NUCLEON MOMENTUM DISTRIBUTIONS

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

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

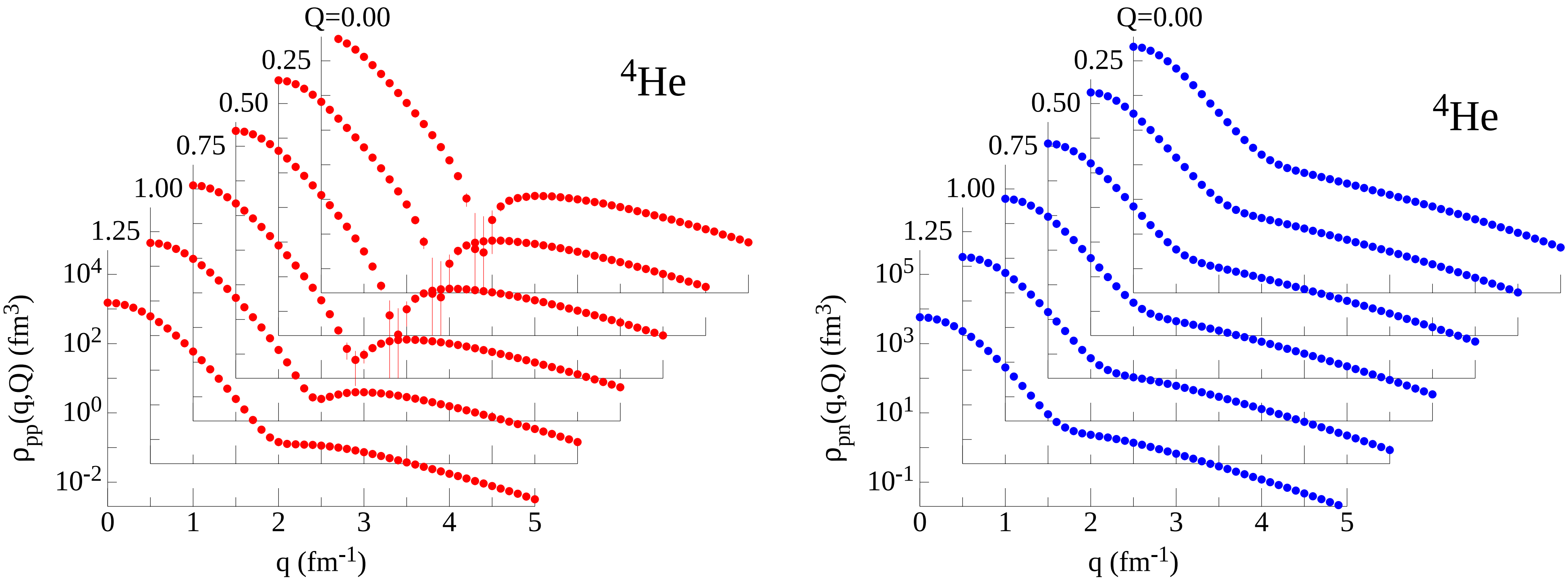
- Useful input for electron scattering studies
- Universal character of high-momentum tails from np tensor interaction



Wiringa, Schiavilla, Pieper, & Carlson, PRC **89**, 024305 (2014)

TWO-NUCLEON MOMENTUM DISTRIBUTIONS

Probability $\rho_{NN}(q,Q)$ of finding a pair of nucleons with relative momentum q and total momentum Q can be defined in a similar fashion:



- Large ratio $\rho_{pn}(q,Q=0)$ / $\rho_{pp}(q,Q=0)$ has been observed in ^{12}C$(e,e'pN)$ scattering
- Results in good agreement with recent ^{4}He$(e,e'pN)$ experiment

Korover, *et al.* (JLab Hall A), PRL **113**, 022501 (2014)

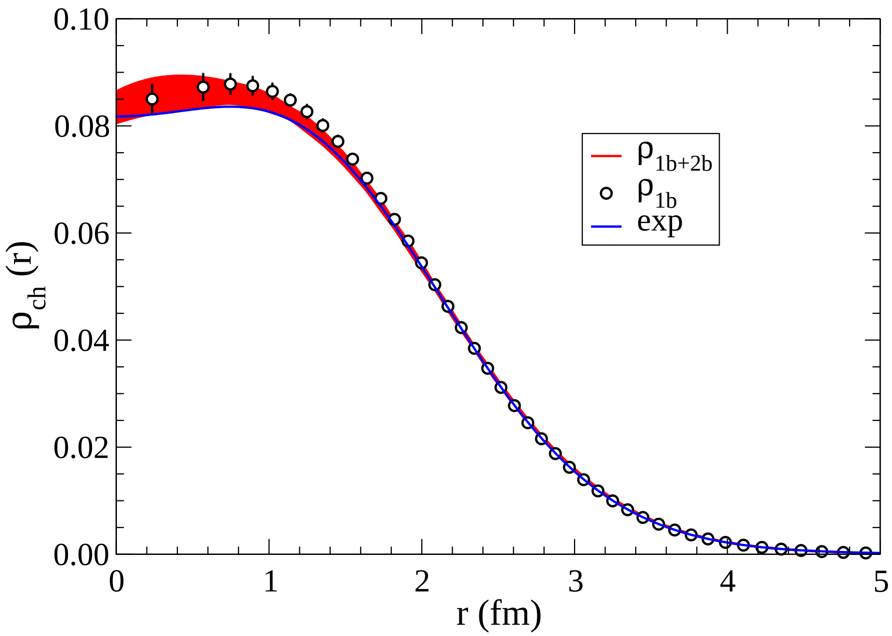
MAKING GFMC WORK ON 786,432 PROCESSORS AND ^{12}C

UNEDF & NUCLEI SciDAC grants to develop general-purpose load-balancing library (ADLB) to run under MPI on 49,152 nodes with OpenMP for 16 cores/node

INCITE grant of Argonne BG/P & Q time used for ^{12}C calculations

- AV18+IL7 Hamiltonian
- Ψ_V has 3-α structure and complete set of 0^+ p-shell states
- GFMC generates central density dip
- Form factor and sum rules in good agreement with experiment

	VMC	GFMC	Expt.
E (MeV)	–65.8(2)	–93.3(4)	–92.16
$\langle r^2\rangle^{1/2}$ (fm)	2.36	2.35	2.33



Lusk, Pieper, & Butler, SciDAC Review Spring 2010

Lovato, Gandolfi, Butler, Carlson, Lusk, Pieper, & Schiavilla, PRL **111**, 092501 (2013)

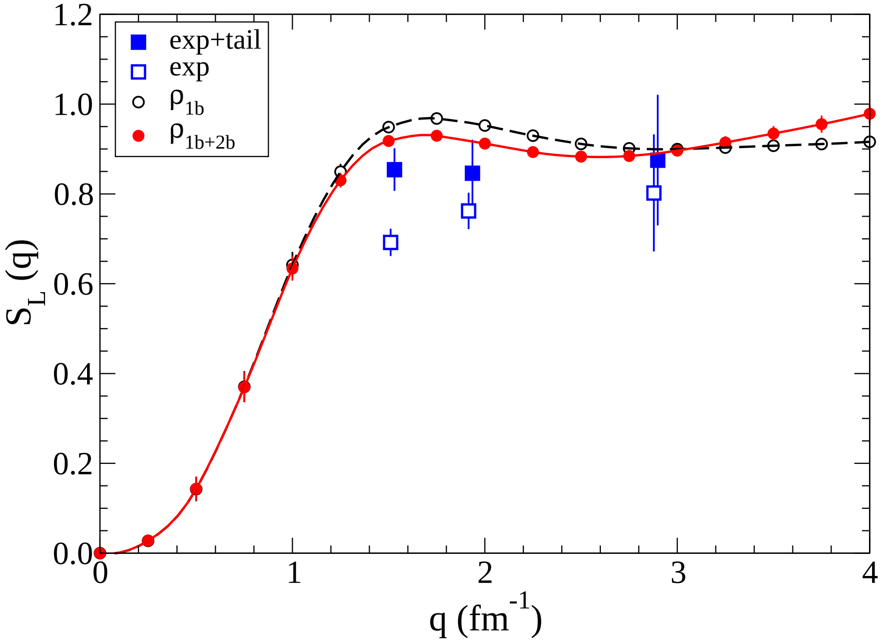
ELECTROWEAK SUM RULES FOR ^{12}C

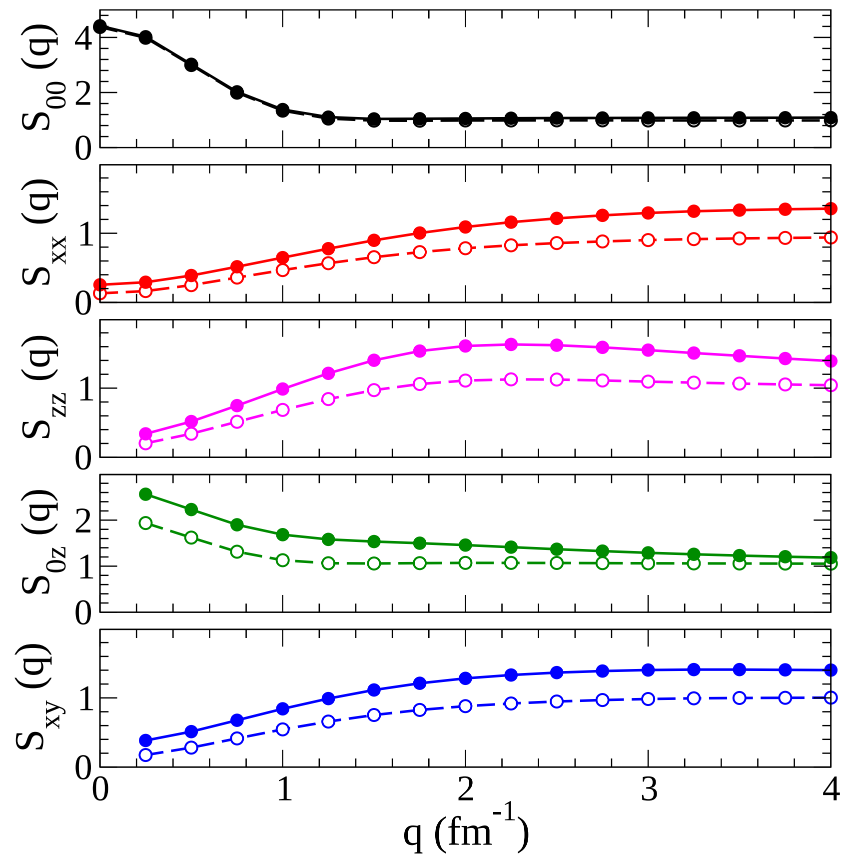
Coulomb longitudinal and transverse sum rules for inclusive (e, e') scattering

Neutral weak current sum rules for inclusive neutrino scattering

$$S_\alpha(q) = C_\alpha \int_{\omega_{\rm th}^+}^{\infty} {\rm d}\omega \, \frac{R_\alpha(q,\omega)}{G_E^{p\,2}(Q^2)}$$

$$C_L = \frac{1}{Z} \,, \quad C_T = \frac{2}{\left(Z\,\mu_p^2 + N\,\mu_n^2\right)} \frac{m^2}{q^2}$$





A theory that reproduces e scattering is the best predictor for ν scattering

Lovato, Gandolfi, Carlson, Pieper, & Schiavilla, PRL **112**, 182502 (2014)

Conclusions

We have demonstrated that realistic nuclear Hamiltonians and currents with 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
- Produce spectroscopic overlaps, ANCs, widths for application to low-energy reactions

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 ^{9,10,11,12}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, widths for $\langle (A\text{-}4)\alpha | A \rangle$

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

- cluster VMC for ^{16}O, ^{40}Ca (done in 1990s and now being revived)
- exascale computing for ^{16}O ($\sim 1000\times$ more expensive than ^{12}C)
- AFDMC (auxiliary field diffusion Monte Carlo) or hybrid GFMC-AFDMC

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