Quantum Monte Carlo Calculations of Transitions and Reactions

(or, Evaluating Off-Diagonal Matrix Elements)

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Work not possible without extensive computer resources
Argonne Laboratory Computing Resource Center (Fusion & Blues)
Argonne Math. & Comp. Science Division (SiCortex)
Argonne Leadership Computing Facility (BlueGene/P & /Q)

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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

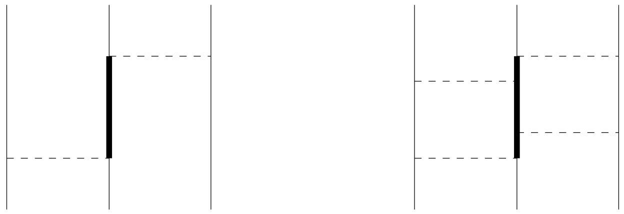
- Two-nucleon potentials that accurately describe elastic NN scattering data
- Consistent three-nucleon potentials and electroweak current operators
- Accurate methods for solving the many-nucleon Schrödinger equation

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

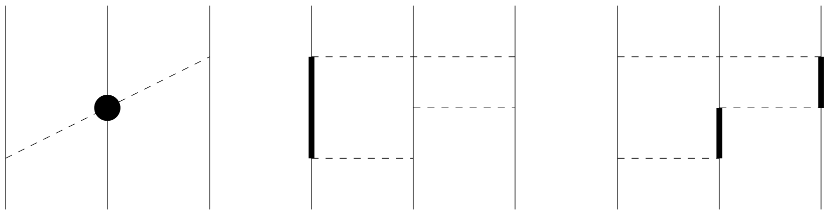
THREE-NUCLEON POTENTIALS

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

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

- 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 steps $\Delta\tau$

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

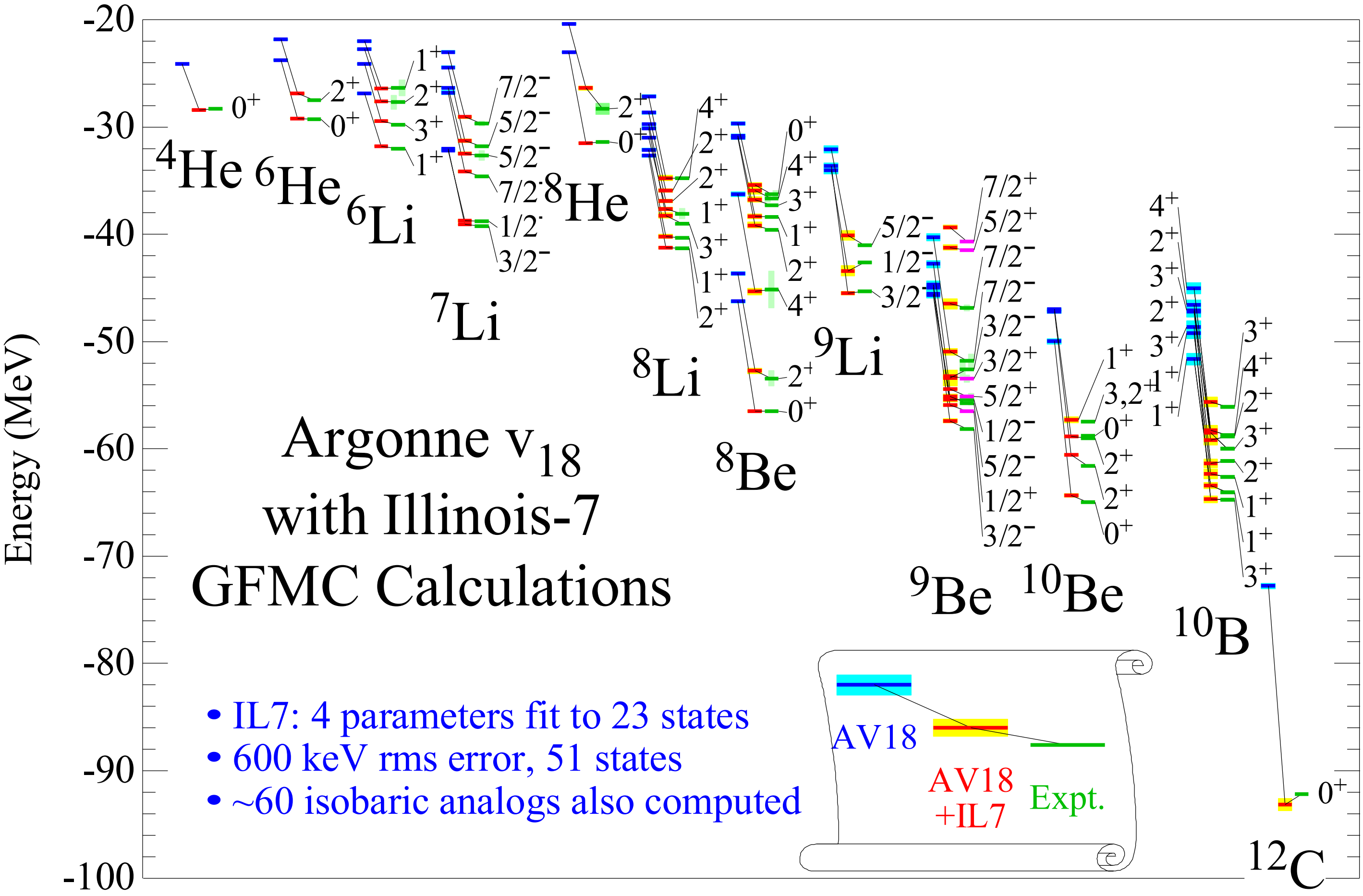
Mixed estimates used for expectation values

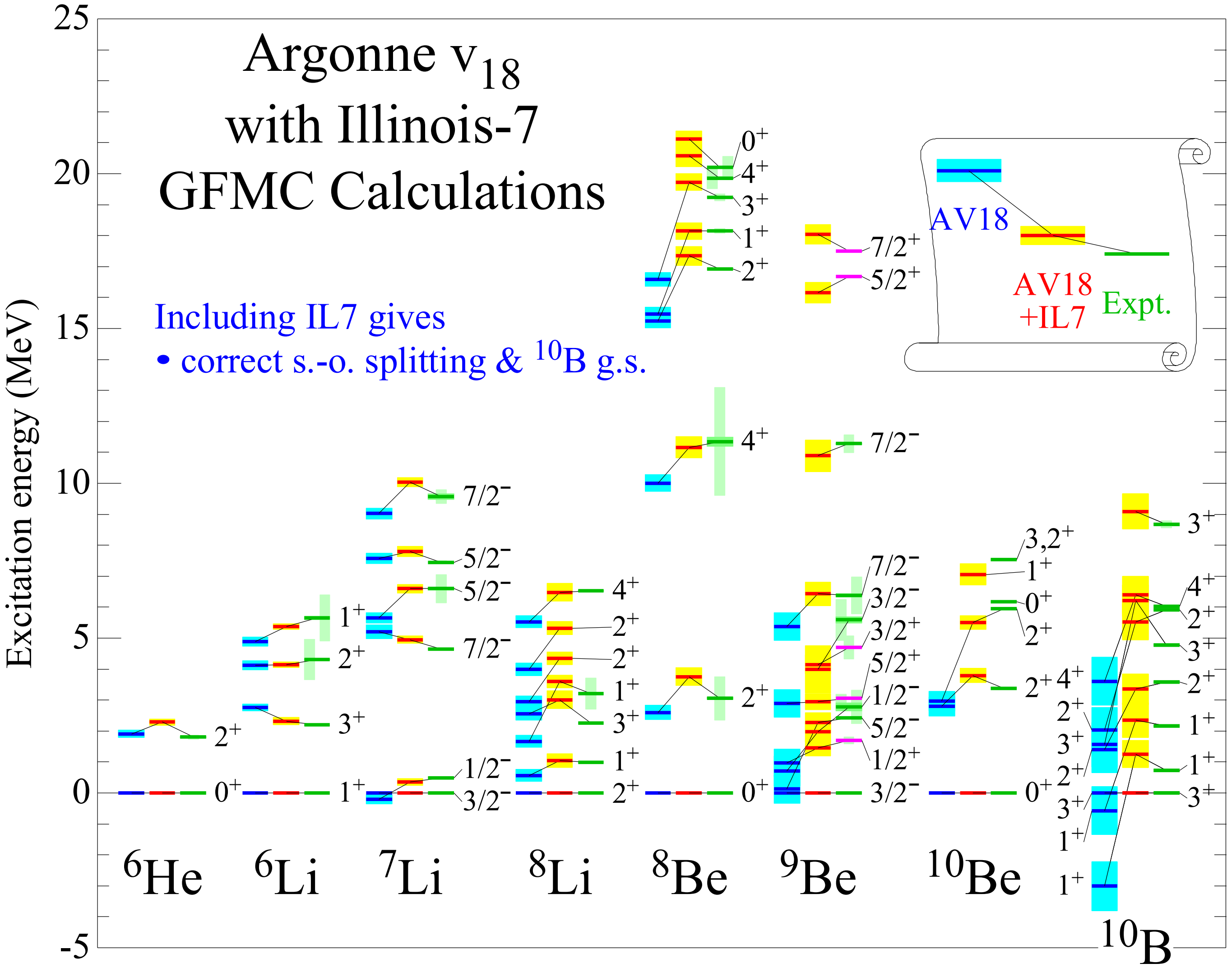
$$\langle O(\tau)\rangle = \frac{\langle \Psi(\tau)|O|\Psi(\tau)\rangle}{\langle \Psi(\tau)|\Psi(\tau)\rangle} \approx \langle O(\tau)\rangle_{\mathrm{Mixed}} + [\langle O(\tau)\rangle_{\mathrm{Mixed}} - \langle O\rangle_V]$$

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

- Cannot propagate p^2, L^2, or $(\mathbf{L}\cdot\mathbf{S})^2$ operators $\Rightarrow$ use $H' = \mathrm{AV8}' + \tilde{V}_{ijk}$
- 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)
Pieper, Wiringa, & Carlson, PRC **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)
6He
6Li
7Li
8Li
8Be
9Be
10Be
10B

M 1, E 2, F, GT transitions

NO EFFECTIVE CHARGES!

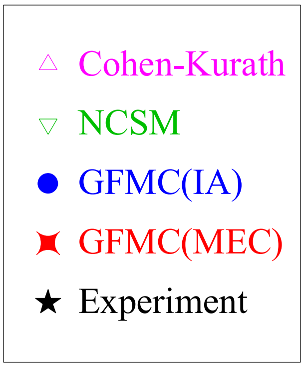
$$E2 = e \sum_k \tfrac{1}{2} r_k^2 Y_2(\hat{r}_k)\,(1+\tau_{kz})$$

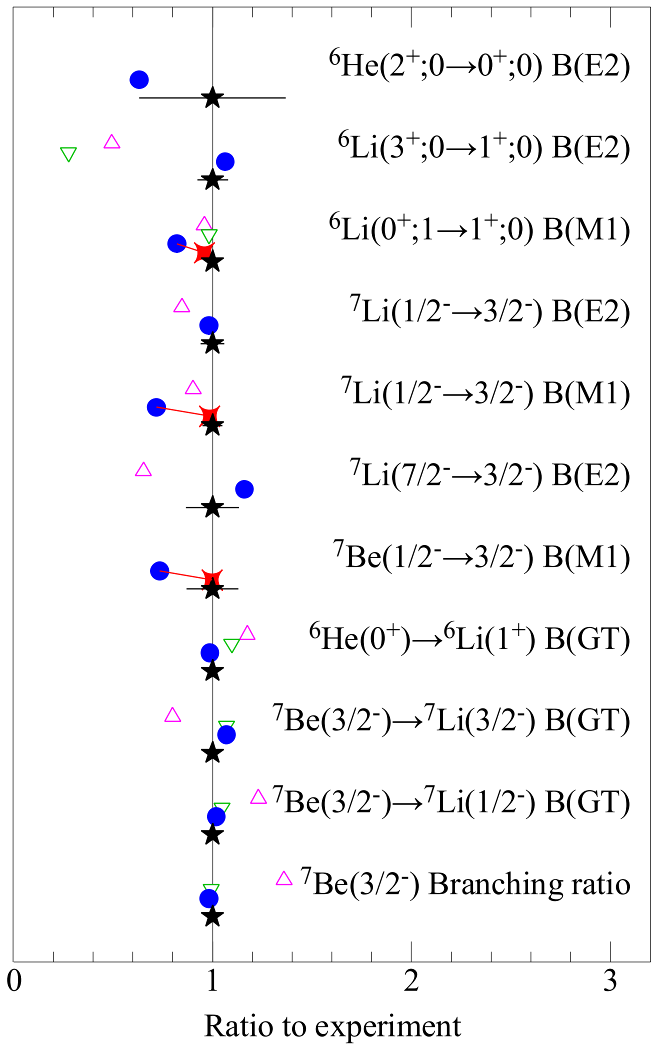
$$M1 = \mu_N \sum_k [(L_k + g_p S_k)(1+\tau_{kz})/2 + g_n S_k\,(1-\tau_{kz})/2]$$

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

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

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

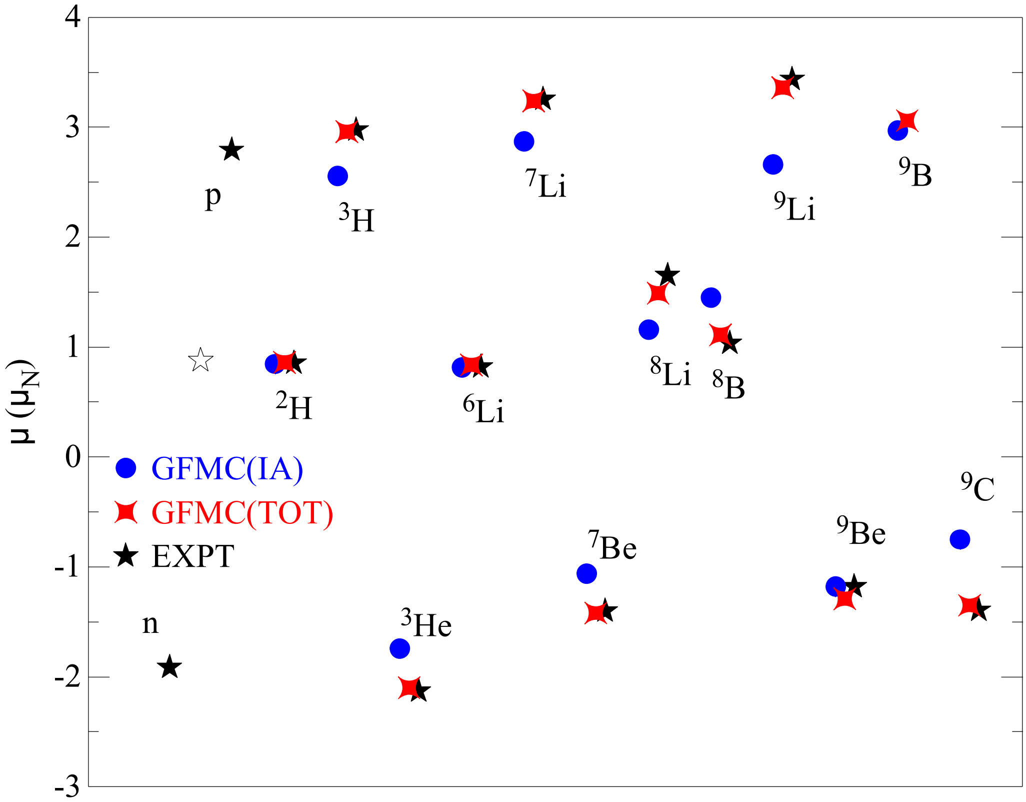




Magnetic moments w/ χEFT exchange currents

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)

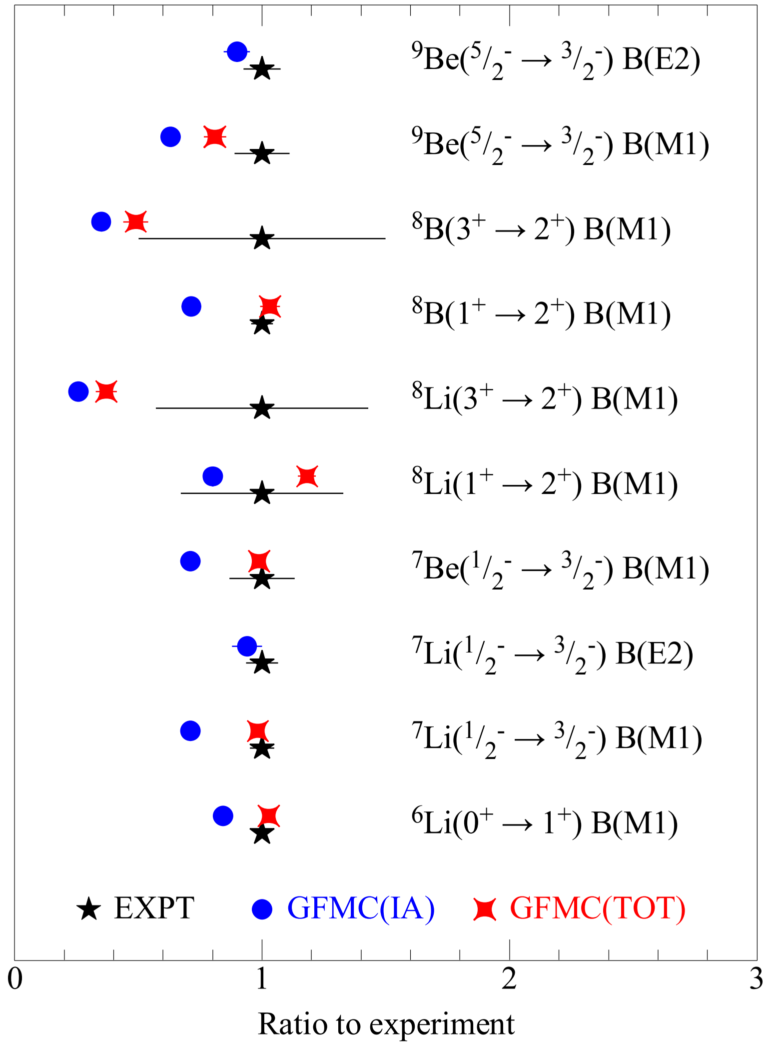


M 1 TRANSITIONS W/ χEFT

- 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 μ_{S} (^{3}H/^{3}He)
- c^{V} is fit to experimental μ_{V} (^{3}H/^{3}He)
- $\Lambda = 600$ MeV

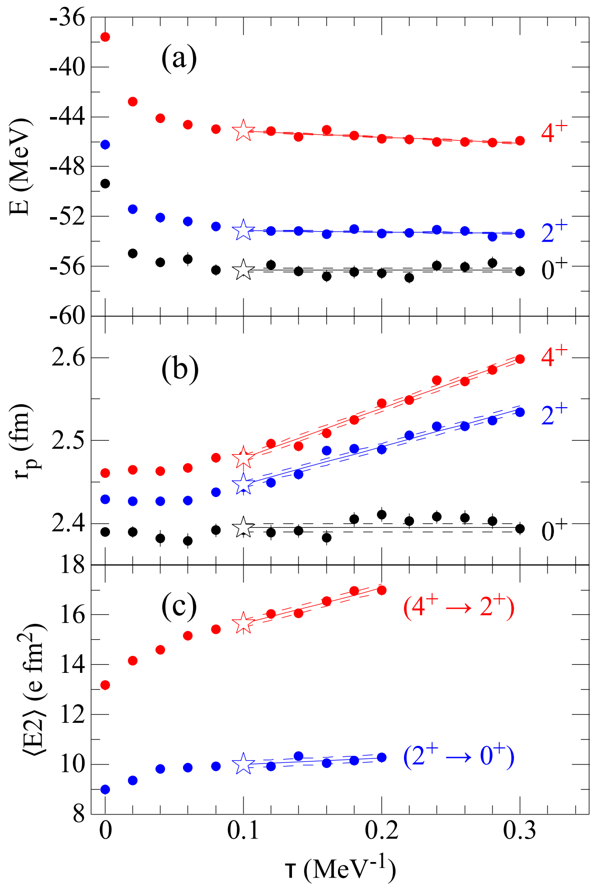
Pastore, Pieper, Schiavilla, & Wiringa

PRC **87**, 035503 (2013)



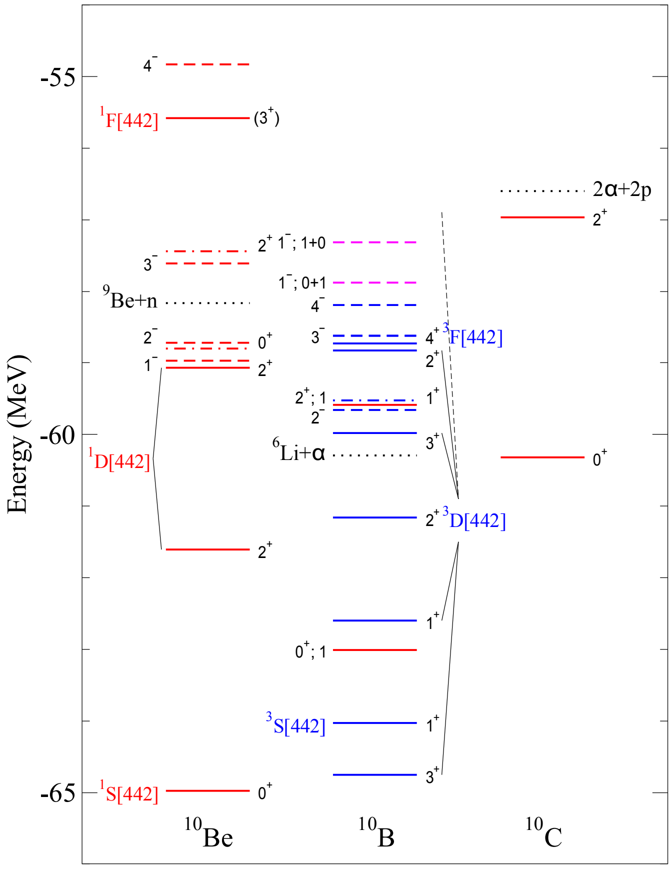
E2 TRANSITIONS IN ^{8}BE

- New experiment at Bhabha Atomic Research Centre 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 τ = 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

The Challenge of A=10 Nuclei

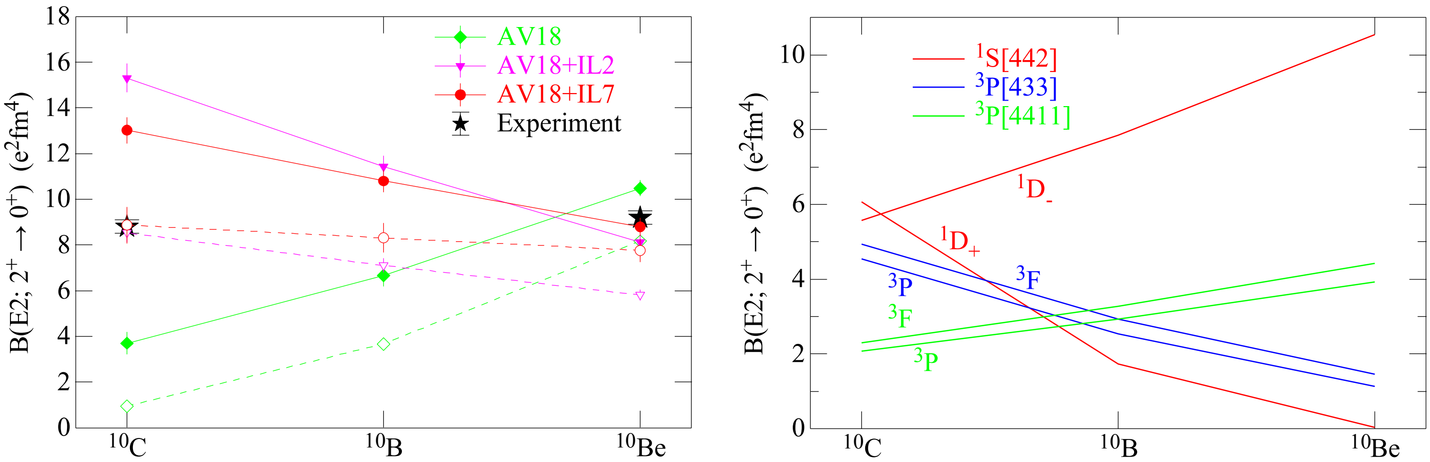


- ^{10}Be & ^{10}B are the lightest nuclei with multiple stable excited states
- At mid-shell there are two linearly independent ^{1}D[442] symmetry states in ^{10}Be and two sets of ^{3}D[442] states in ^{10}B differentiated by +/- quadrupole moments
- Early GFMC calcs in ^{10}Be with AV18 and AV18+UIX get degenerate energies for the two 2^+ states
- Later GFMC calcs with AV18+IL2 and AV18+IL7 get the negative quadrupole state lower
- How can experiment tell us which state is which?

PRECISE EXPERIMENTAL TESTS OF THE ELECTROMAGNETIC RATES

New measurements of the lifetimes of the two ^{10}Be 2^+ states were made using the Doppler shift attenuation method following the ^{7}Li(^{7}Li,α)^{10}Be reaction. The $B(E2\downarrow) = 9.2(3) e^2\text{fm}^4$ for the $J^\pi = 2^+_1$ state and $0.11(2) e^2\text{fm}^4$ for the $J^\pi = 2^+_2$ state.

A subsequent measurement of the lifetime of the 2^+_1 state in ^{10}C following the $p(^{10}\text{B},n)^{10}$C reaction, got $B(E2\downarrow) = 8.8(3) e^2\text{fm}^4$.



GFMC calculations using AV18 without or with IL2 or IL7 all get the 2^+_1 transition in ^{10}Be about right, but give widely varying predictions in ^{10}C. The latter appears much more sensitive to precise mixing of different symmetry state contributions, and thus to details of V_{ijk}.

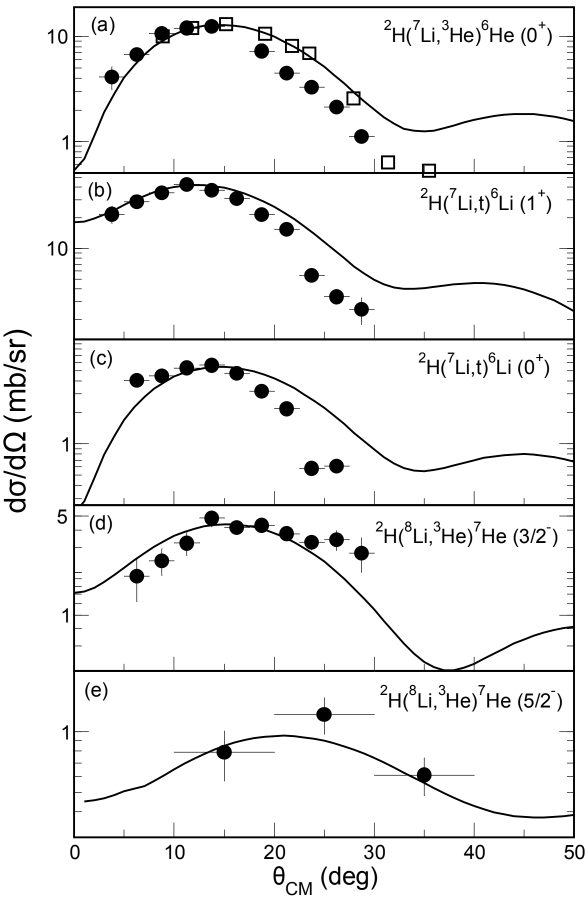
McCutchan, Lister, Wiringa, Pieper, et al., PRL **103**, 192501 (2009) ; PRC **86**, 014312 (2012)

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 $d(^8\mathrm{Li},p)^9\mathrm{Li}$ (ATLAS) & $d(^9\mathrm{Li},t)^8\mathrm{Li}$ (TRIUMF)

- PTOLEMY DWBA calculations for transfer
- (d,p) vertex from AV18
- (d,t), $(^8\mathrm{Li},^9\mathrm{Li})$, 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 $\alpha \equiv [J_A^\pi, T_A, T_{z_A}]$, $\gamma \equiv [J_{A-1}^\pi, T_{A-1}, T_{z_{A-1}}]$, 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:

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

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

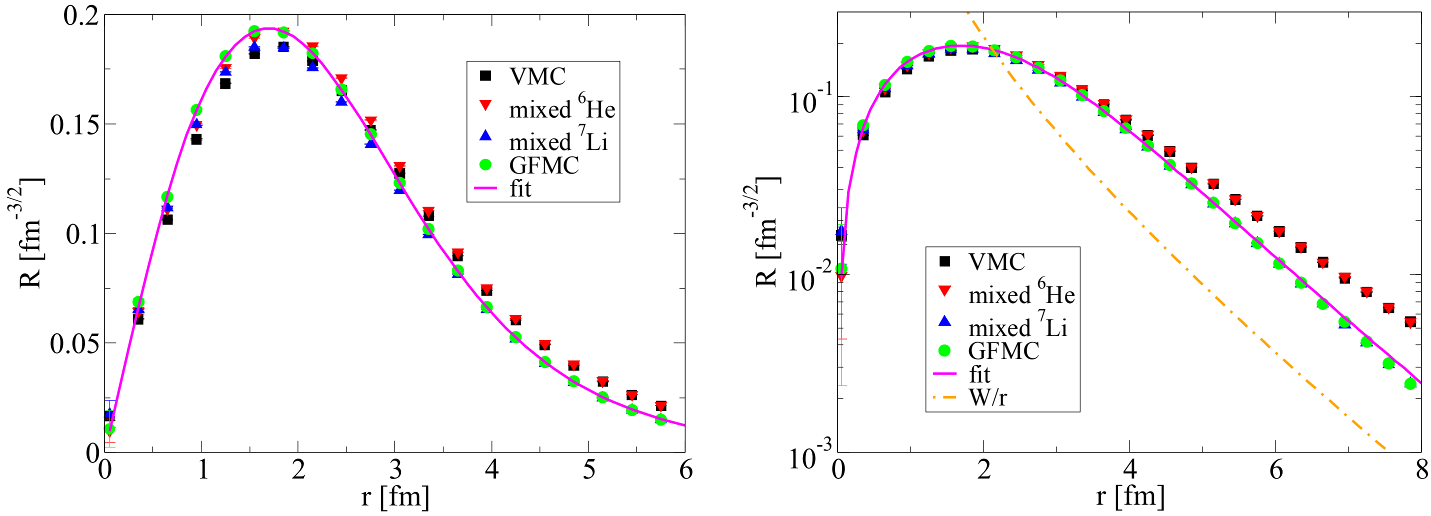
$$R(\alpha,\gamma,\nu;r) \xrightarrow{r\to\infty} C(\alpha,\gamma,\nu)\frac{W_{-\eta,l+1/2}(2kr)}{r},$$

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:

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

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



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

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

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.

An alternative to explicit computation of the overlap function is an integral over the wave function interior:

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

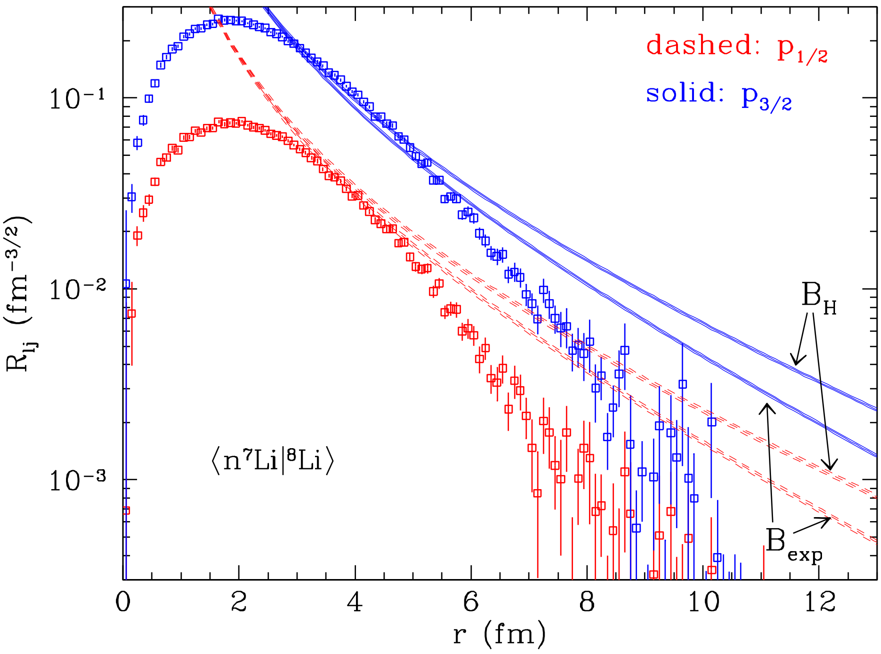
$M_{-\eta,l+\frac{1}{2}}(2kr)$ is the "other" Whittaker function, irregular at $r \to \infty$. Here $U_{\rm rel}$ is

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

and at large separation of the last nucleon, $U_{\rm rel} \to V_C$, so $(U_{\rm rel} - V_C) \to 0$.
This makes the integrand terminate at ~ 7 fm for many p-shell nuclei.

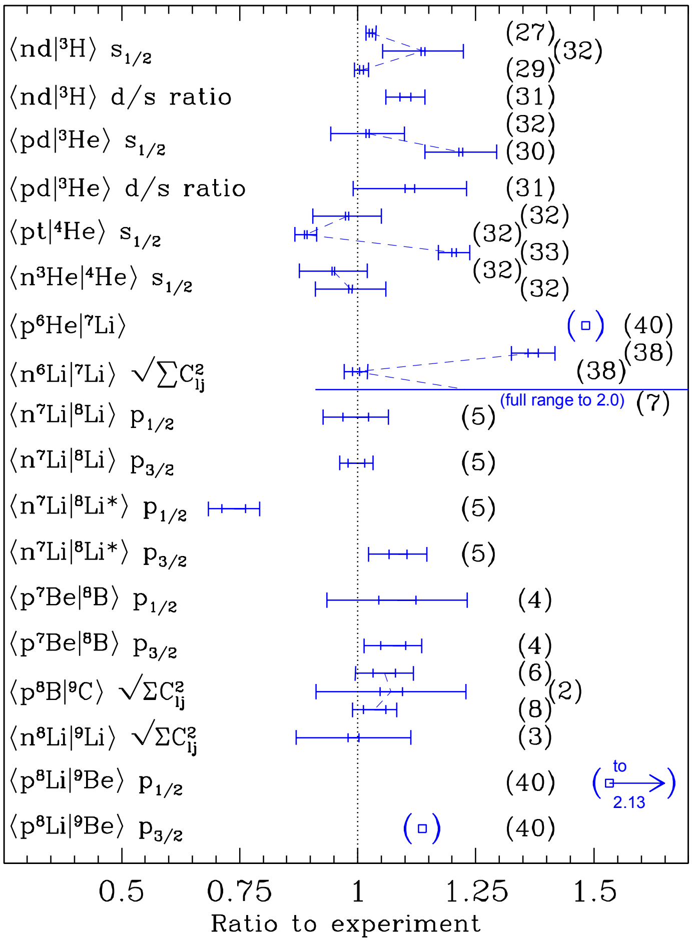
ANC: $^8\text{Li} \rightarrow ^7\text{Li} + n$

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
$C^2_{p\,1/2}$	0.029(2)	0.048(3)	0.048(6)
$C^2_{p\,3/2}$	0.237(9)	0.382(14)	0.384(38)

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 $A > 4$
- $S_{17}(0)$=[38.7(eV b fm)]$|C(2^+, {}^8B)|^2$ = 20.8 eV b = Solar fusion II recommended value
- Similar integral relation can give good estimate of excited state widths

Nollett & Wiringa, PRC **83**, 041001(R) (2011)

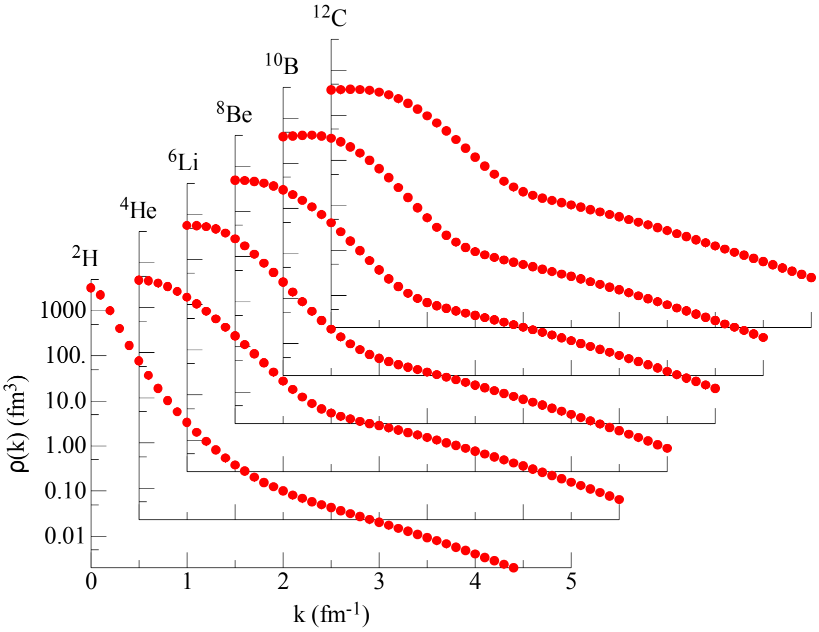
Nollett, PRC **86**, 044330 (2012)

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

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 ^{8}Be isospin-mixing, ^{10}C$(\beta^+)^{10}$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, PRL **99**, 022507 (2007)

HAPPY BIRTHDAY JAMES

!!!