Quantum Monte Carlo Studies of the Structure of Light Nuclei

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Work not possible without extensive computer resources:

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Argonne Math. & Comp. Science Division (BlueGene/L)
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Argonne NATIONAL LABORATORY

Physics Division

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GOAL OF *ab-initio* LIGHT-NUCLEI CALCULATIONS

We seek to understand nuclei as collections of interacting nucleons by reliably solving the many-nucleon Schrödinger equation for realistic Hamiltonians of the form

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

Using quantum Monte Carlo methods we want to compute

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

With accurate calculations we can rigorously test a given Hamiltonian.

At present our methods are limited to light ($A \leq 12$) nuclei
and local potentials with weak quadratic-momentum dependence.

ARGONNE V$_{18}$

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

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

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

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

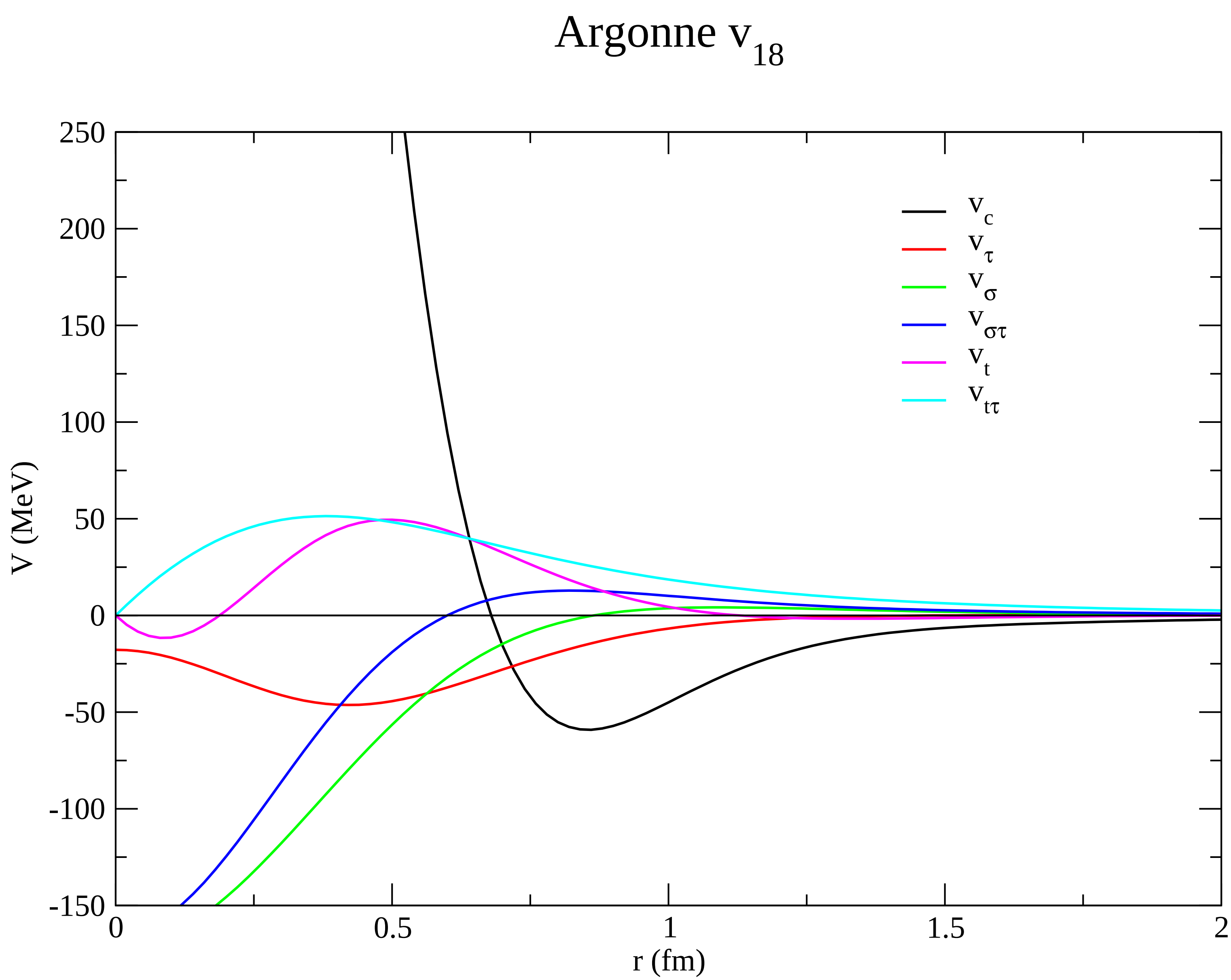
$$v_{ij}^{I} = \sum_p I^p T_\pi^2(r_{ij})O_{ij}^p$$

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

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

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

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 and ^{2}H binding energy

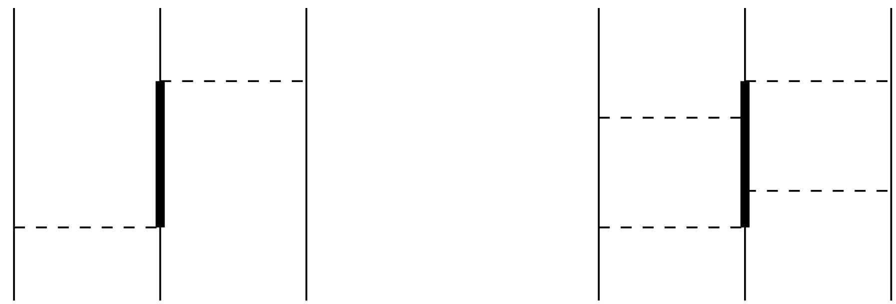


Argonne v18
250
200
150
100
50
0
-50
-100
-150
V (MeV)
0
0.5
1
1.5
2
r (fm)
vc
vτ
vσ
vστ
vt
vtτ

Three-nucleon potentials

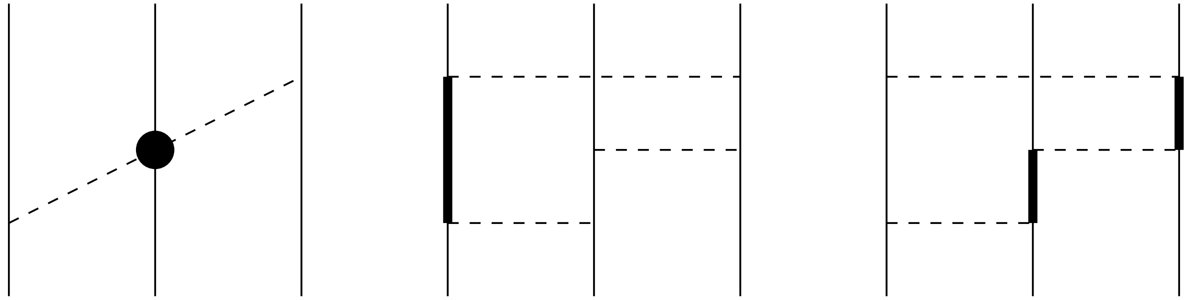
Urbana IX (UIX)

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



Illinois 2 (IL2)

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



The Many-Body Problem

Need to solve

$\mathcal{H}\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_A; t_1, t_2, \cdots, t_A) = E\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_A; s_1, s_2, \cdots, s_A; t_1, t_2, \cdots$

s_i are nucleon spins: $\pm\frac{1}{2}$

t_i are nucleon isospins (proton or neutron): $\pm\frac{1}{2}$

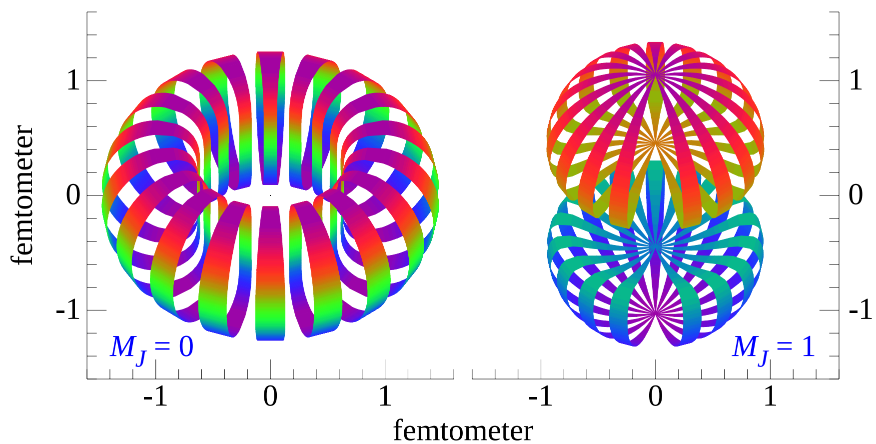
$2^A \times \binom{A}{Z}$ complex coupled 2^{nd} order differential equations in $3A$ dimensions

(number of isospin states can be reduced)

^{12}C: 270,336 coupled equations in 36 dimensions

Coupling is strong:

- $\langle v_{\text{tensor}} \rangle$ is $\sim 60\%$ of total $\langle v_{ij} \rangle$
- $\langle v_{\text{tensor}} \rangle = 0$ if no tensor correlations



Variational Monte Carlo

Minimize expectation value of H

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

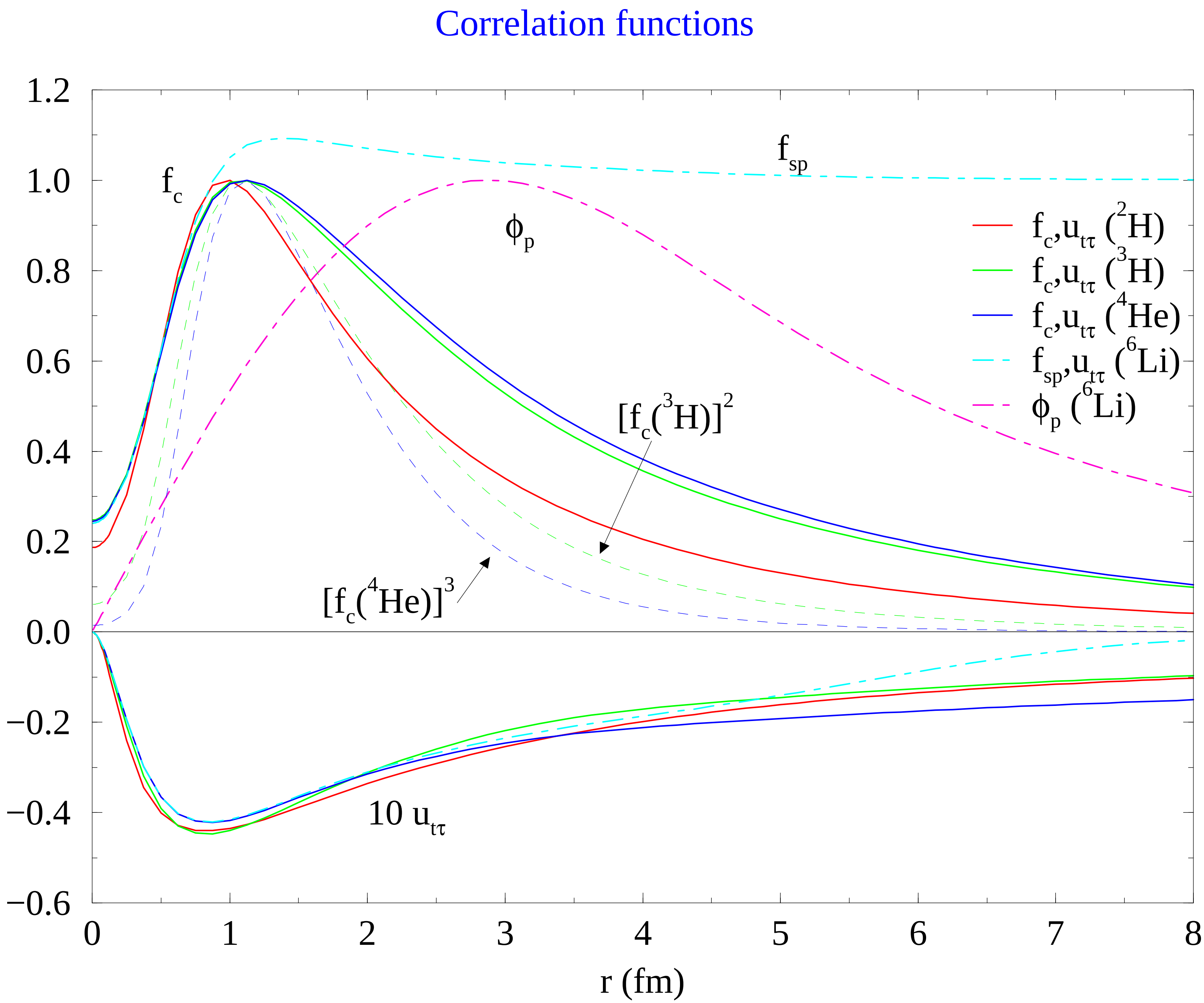
Trial function (s-shell nuclei)

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

$$|\Phi_d(1100)\rangle = \mathcal{A} | \uparrow p \uparrow n \rangle \;\; ; \;\; |\Phi_\alpha(0000)\rangle = \mathcal{A} | \uparrow p \downarrow p \uparrow n \downarrow n \rangle$$

$$U_{ij} = \sum_{p=2,6} u_p(r_{ij}) O_{ij}^p \;\; ; \;\; U_{ijk}^{TNI} = -\epsilon V_{ijk}(\tilde{r}_{ij}, \tilde{r}_{jk}, \tilde{r}_{ki})$$

Functions $f_c(r_{ij})$ and $u_p(r_{ij})$ are obtained numerically from solution of coupled differential equations containing v_{ij} .



Correlation functions
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
1
2
3
4
5
6
7
8
r (fm)
f_c
f_{sp}
ϕ_p
$f_c,u_{t\tau}$ (^{2}H)
$f_c,u_{t\tau}$ (^{3}H)
$f_c,u_{t\tau}$ (^{4}He)
$f_{sp},u_{t\tau}$ (^{6}Li)
ϕ_p (^{6}Li)
$[f_c(^3H)]^2$
$[f_c(^4He)]^3$
10 $u_{t\tau}$

Trial function (p-shell nuclei)

$$\Rightarrow \quad \mathcal{A}\left\{ \prod_{i<j\leq 4} f_{ss}(r_{ij}) \sum_{LS[n]} \Big(\beta_{LS[n]} \prod_{k\leq 4<l\leq A} f_{sp}(r_{kl}) \prod_{4<l<m\leq A} f_{pp}(r_{lm}) \right.$$

$$\left. |\Phi_\alpha(0000)_{1234} \prod_{4<l\leq A} \phi_p^{LS[n]}(R_{\alpha l}) \left\{ [Y_1^{m_l}(\Omega_{\alpha l})]_{LM_L} \otimes [\chi_l(\tfrac{1}{2}m_s)]_{SM_S} \right\}_{JM} [\nu_l(\tfrac{1}{2}t_3)]_{TT_3} \rangle \right\}$$

Permutation symmetry

A	$[n]$	L	(T,S)
6	[2]	0, 2	(1, 0), (0, 1)
	[11]	1	(1, 1), (0, 0)
7	[3]	1, 3	(1/2, 1/2)
	[21]	1, 2	(3/2, 1/2), (1/2, 3/2), (1/2, 1/2)
	[111]	0	(3/2, 3/2), (1/2, 1/2)
8	[4]	0, 2, 4	(0, 0)
	[31]	1, 2, 3	(1, 1), (1, 0), (0, 1)
	[22]	0, 2	(2, 0), (1, 1), (0, 2), (0, 0)
	[211]	1	(2, 1), (1, 2), (1, 1), (1, 0), (0, 1)

Diagonalization

in $\beta_{LS[n]}$ basis to produce energy spectra $E(J^\pi_x)$ and orthogonal excited states $\Psi_V(J^\pi_x)$

Expectation values

$\Psi_V(\mathbf{R})$ represented by vector with $2^A \times \binom{A}{Z}$ spin-isospin components for each space configuration $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A)$; Expectation values are given by summation over samples drawn from probability distribution $W(\mathbf{R}) = |\Psi_P(\mathbf{R})|^2$:

$$\frac{\langle \Psi_V | O | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} = \sum \frac{\Psi^\dagger_V(\mathbf{R}) O \Psi_V(\mathbf{R})}{W(\mathbf{R})} / \sum \frac{\Psi^\dagger_V(\mathbf{R}) \Psi_V(\mathbf{R})}{W(\mathbf{R})}$$

$\Psi^\dagger \Psi$ is a dot product and $\Psi^\dagger O \Psi$ a sparse matrix operation.

Scaling of calculation

	A	P	$N_S \times N_T$	$\prod(\times^8\text{Be})$
^{4}He	4	6	16×2	0.001
^{6}Li	6	15	64×5	0.036
^{8}Be	8	28	256×14	1.
^{10}B	10	45	1024×42	24.
^{12}C	12	66	4096×132	530.

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 $\Delta\tau$

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

using the short-time propagator accurate to order $(\Delta\tau)^3$

$$G_{\alpha\beta}(\mathbf{R}, \mathbf{R}') = e^{E_0 \delta\tau} G_0(\mathbf{R}, \mathbf{R}') \langle\alpha| \left[\mathcal{S} \prod_{i<j} \frac{g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})} \right] |\beta\rangle$$

where the free many-body propagator is

$$G_0(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R} | e^{-K \triangle\tau} | \mathbf{R}' \rangle = \left[\sqrt{\frac{m}{2\pi\hbar^2 \triangle\tau}} \right]^{3A} \exp\left[\frac{-(\mathbf{R} - \mathbf{R}')^2}{2\hbar^2 \triangle\tau / m} \right]$$

and $g_{0,ij}$ and g_{ij} are the free and exact two-body propagators

$$g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \langle \mathbf{r}_{ij} | e^{-H_{ij} \triangle\tau} | \mathbf{r}'_{ij} \rangle$$

Mixed estimates

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

$$\langle H(\tau)\rangle_{\rm Mixed} = \frac{\langle\Psi(\tau/2)|H|\Psi(\tau/2)\rangle}{\langle\Psi(\tau/2)|\Psi(\tau/2)\rangle} \geq E_0$$

Propagator cannot contain p^2, L^2, or $(\mathbf{L}\cdot\mathbf{S})^2$ operators:

$G_{\beta\alpha}(\mathbf{R}',\mathbf{R})$ has only v_8'

$\langle v_{18} - v_8'\rangle$ computed perturbatively with extrapolation (small for AV18)

Reliable in Faddeev (^{3}H), hyperspherical harmonic & Yakubovsky (^{4}He) comparisons

Fermion sign problem limits maximum τ:

$G_{\beta\alpha}(\mathbf{R}',\mathbf{R})$ brings in lower-energy boson solution

$\langle\Psi_T|H|\Psi(\tau)\rangle$ projects back fermion solution

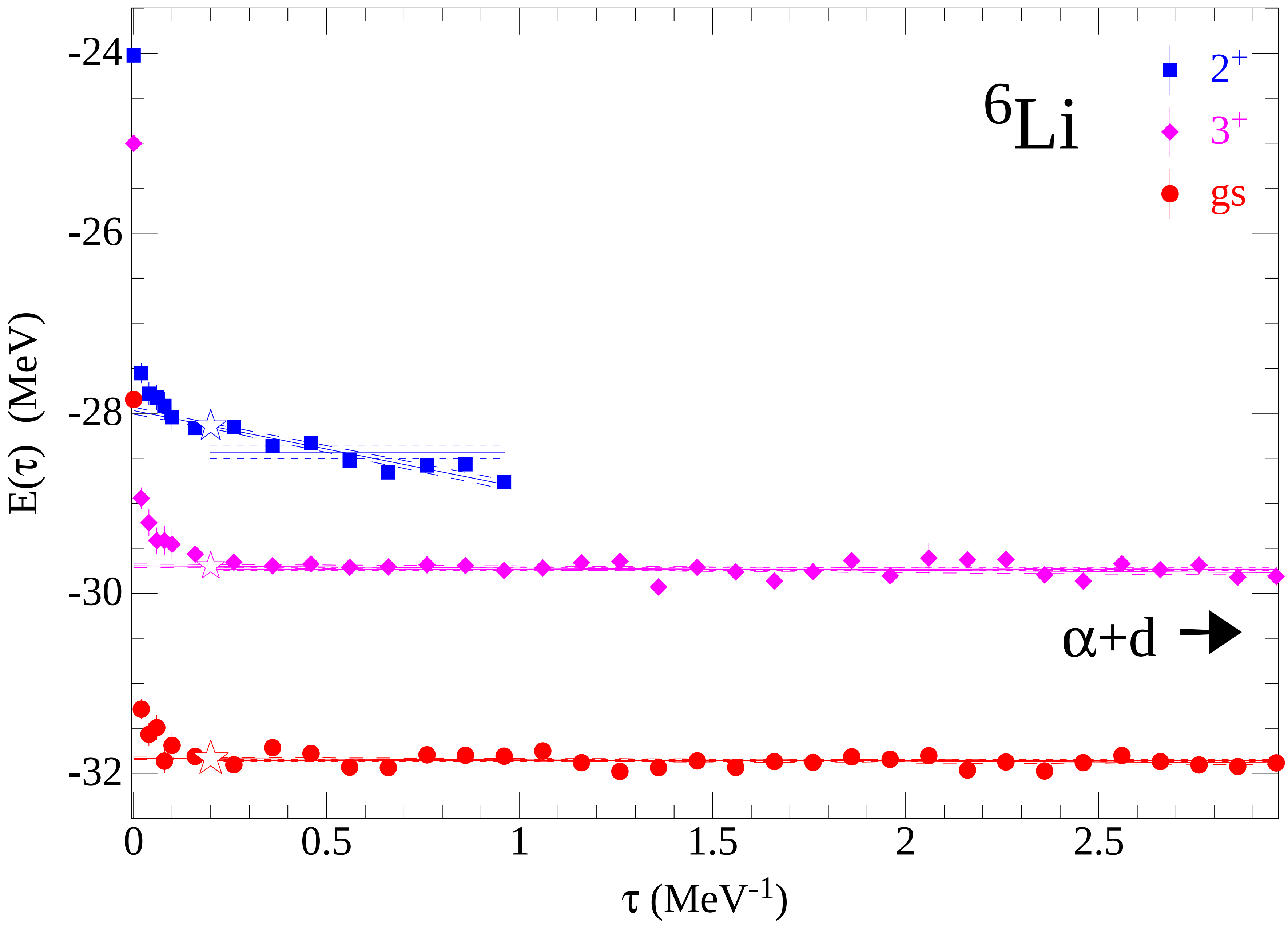
Exponentially growing statistical errors

Constrained-path propagation, removes steps that have

$$\overline{\Psi^\dagger(\tau,\mathbf{R})\Psi(\mathbf{R})} = 0$$

Possible systematic errors reduced by $10-20$ unconstrained steps before evaluating observables.

GFMC propagation of three states in ^{6}Li



GFMC for Second Excited States of same J^π

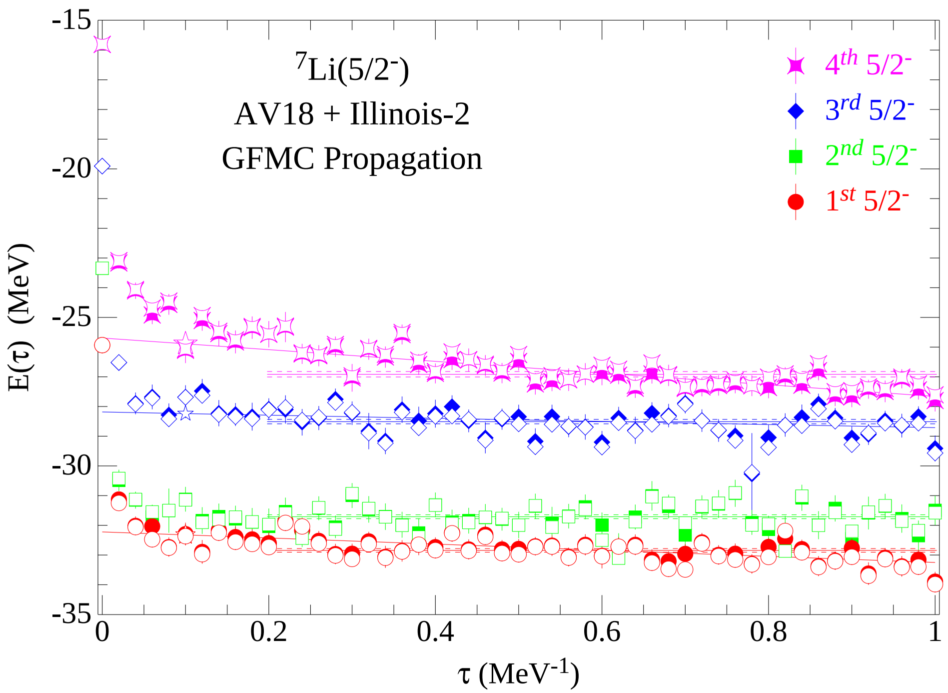
The Ψ_T are constructed by non-orthogonal basis diagonalization in p-shell wave functions.

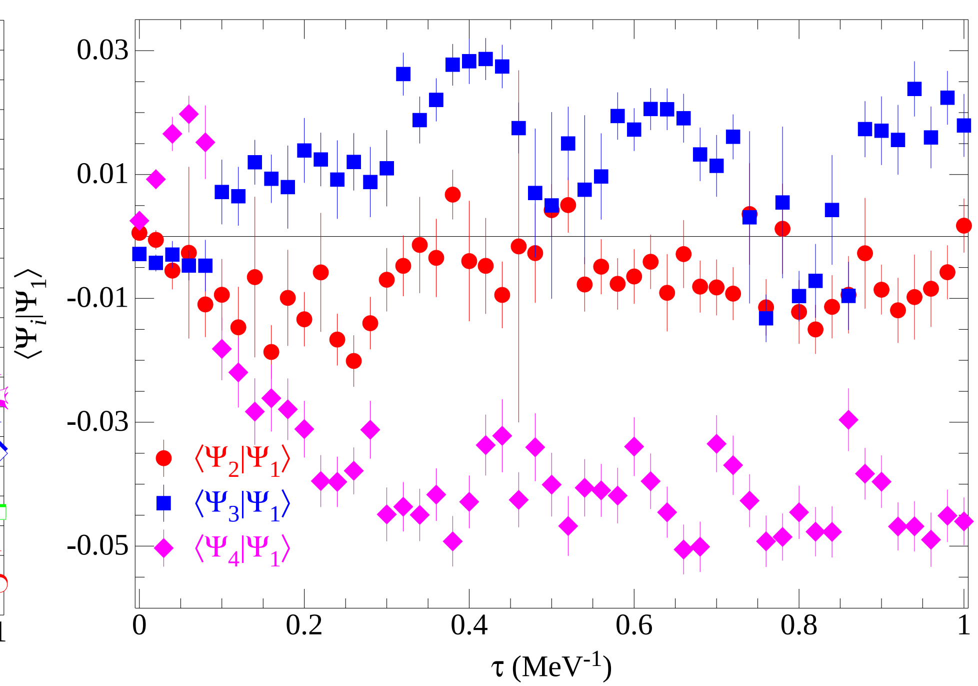
Example: ^{7}Li(5/2-) has 4 symmetry possibilities: ^{2}F[43] , ^{4}P[421] , ^{4}D[421] , ^{2}D[421]

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

Will $e^{-(H-E_0)\tau}\Psi_T(2^{nd}\frac{5}{2}^-) \longrightarrow \Psi_{\rm GFMC}(1^{st}\frac{5}{2}^-)$?

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

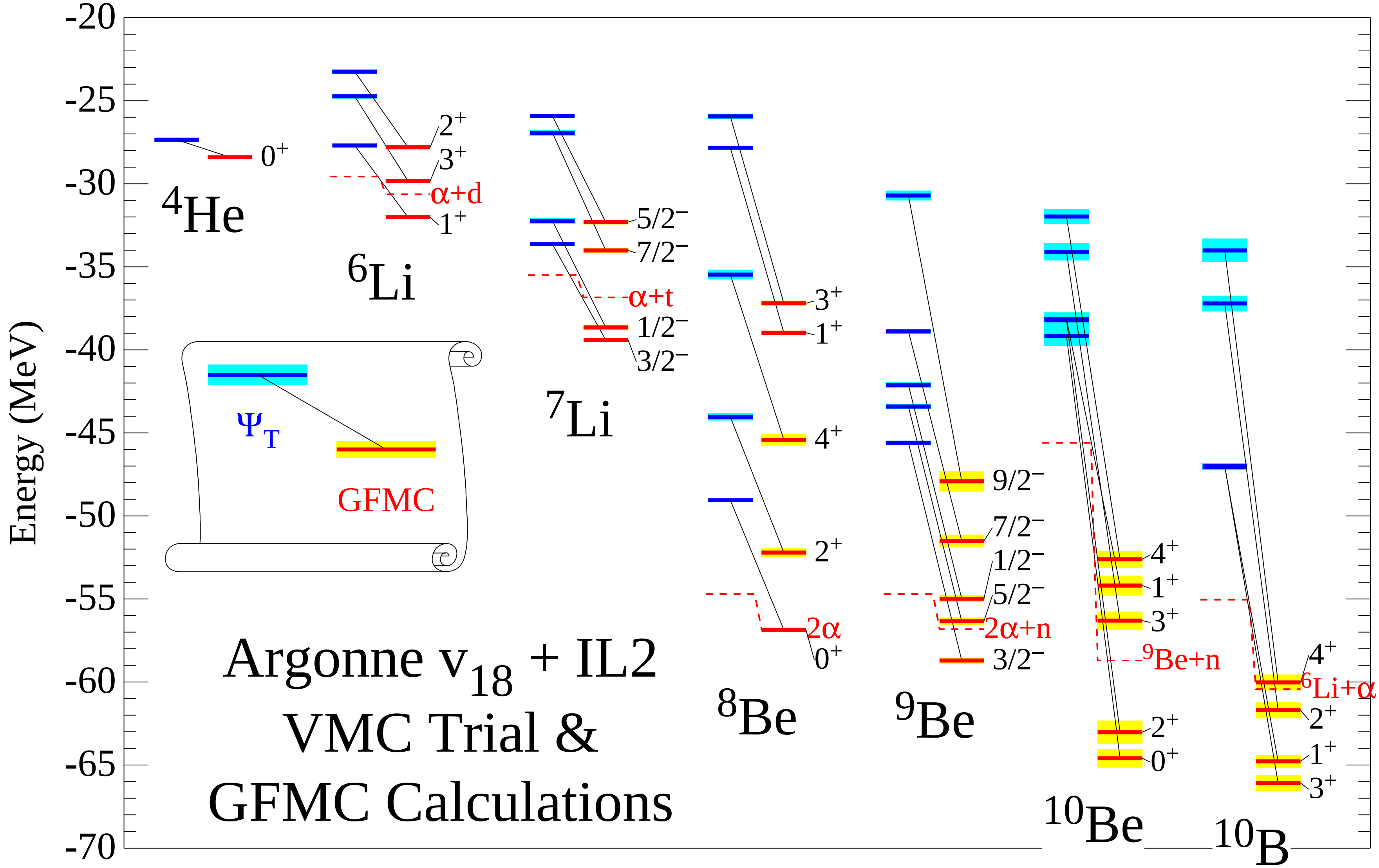




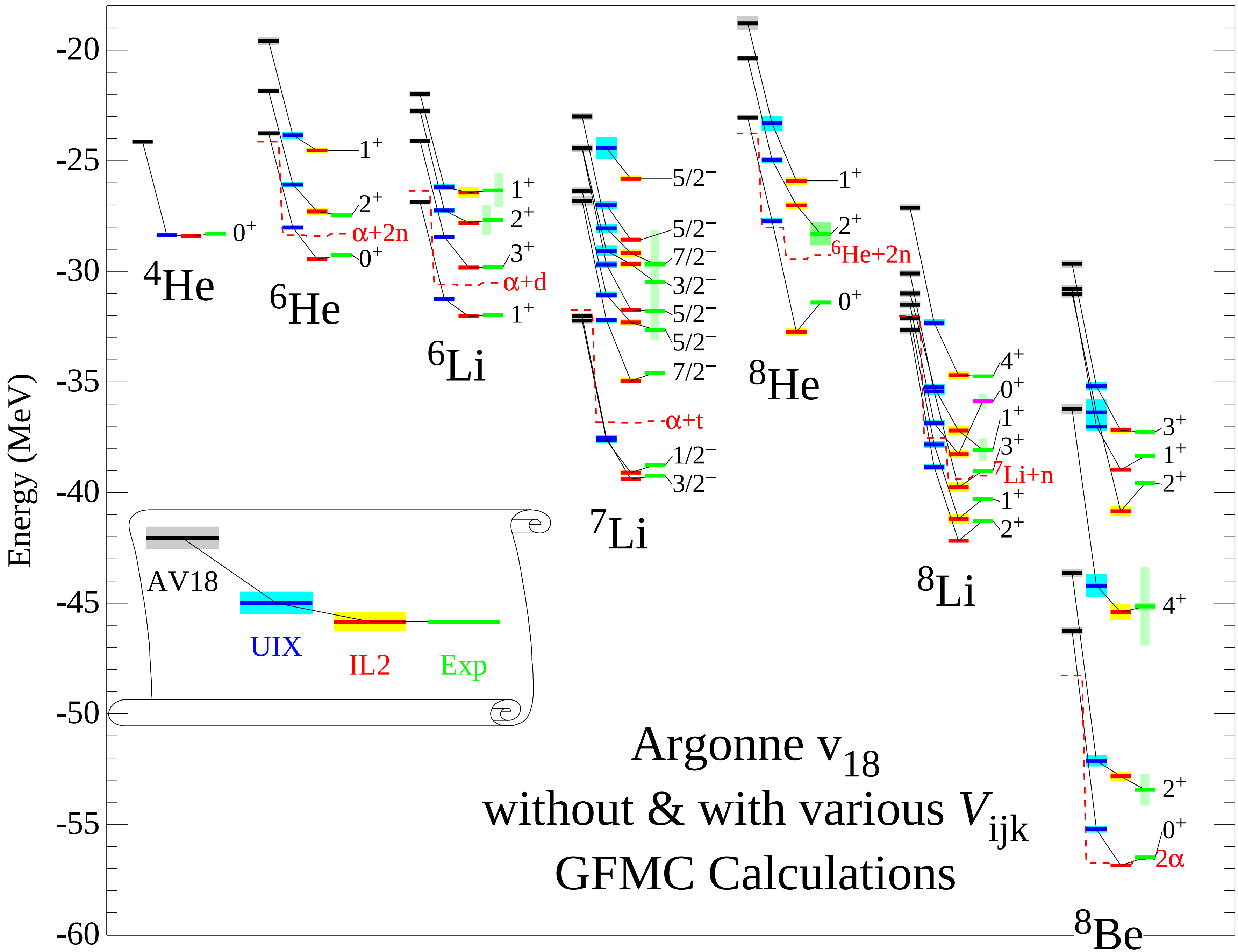
Binding energy results for A=3,4

Hamiltonian	Method	^{3}H	^{3}He	^{4}He
Argonne v_8'	VMC*			25.44(2)
(no EM)	GFMC[1]			25.93(2)
	FY[2]			25.94(5)
	HH[3]			25.90(1)
	SVM[4]			25.92
	EIHH[5]			25.944(10)
	CRCGV[6]			25.90
	NCSM[7]			25.80(20)
Argonne v_{18}	VMC*	7.50(1)	6.77(1)	23.70(2)
	GFMC[1]	7.61(1)	6.89(1)	24.07(4)
	F/FY[2]	7.623	6.924	24.28
	PHH/HH[3]	7.623	6.925	24.18
Argonne v_{18}	VMC*	8.31(1)	7.56(1)	27.72(2)
+ Urbana IX	GFMC[1]	8.46(1)	7.70(1)	28.33(2)
	F/FY[2]	8.478	7.760	28.50
	PHH/CHH[3]	8.480	7.749	28.46
Experiment		8.482	7.718	28.296

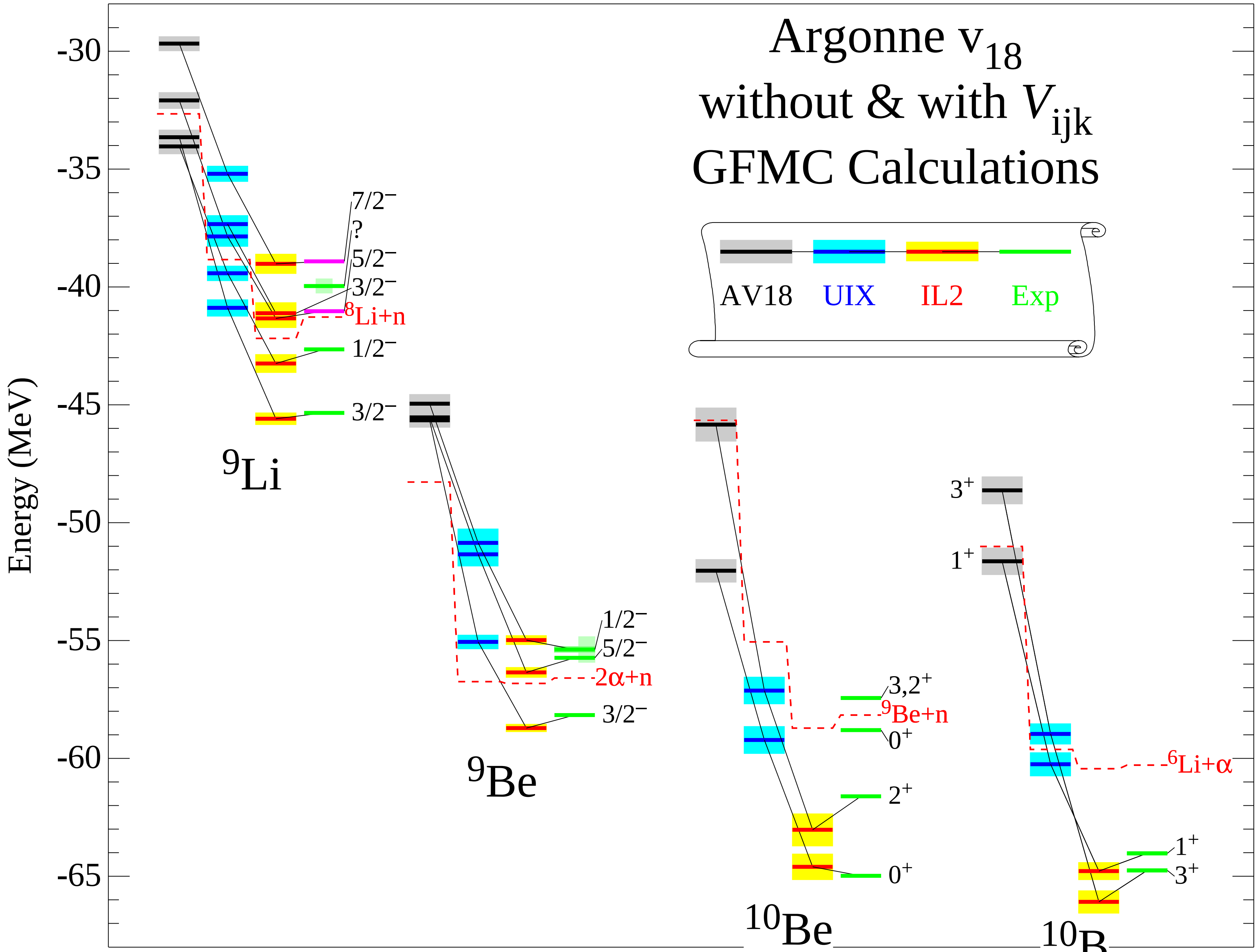
* Arriaga, Pandharipande, Wiringa [1] Carlson, Pieper, Wiringa [2] Kamada, Nogga, Glöckle [3] Viviani, Kievsky, Rosati
[4] Varga, Suzuki [5] Barnea, Leideman, Orlandini [6] Hiyama, Kamimura [7] Navrátil, Barrett



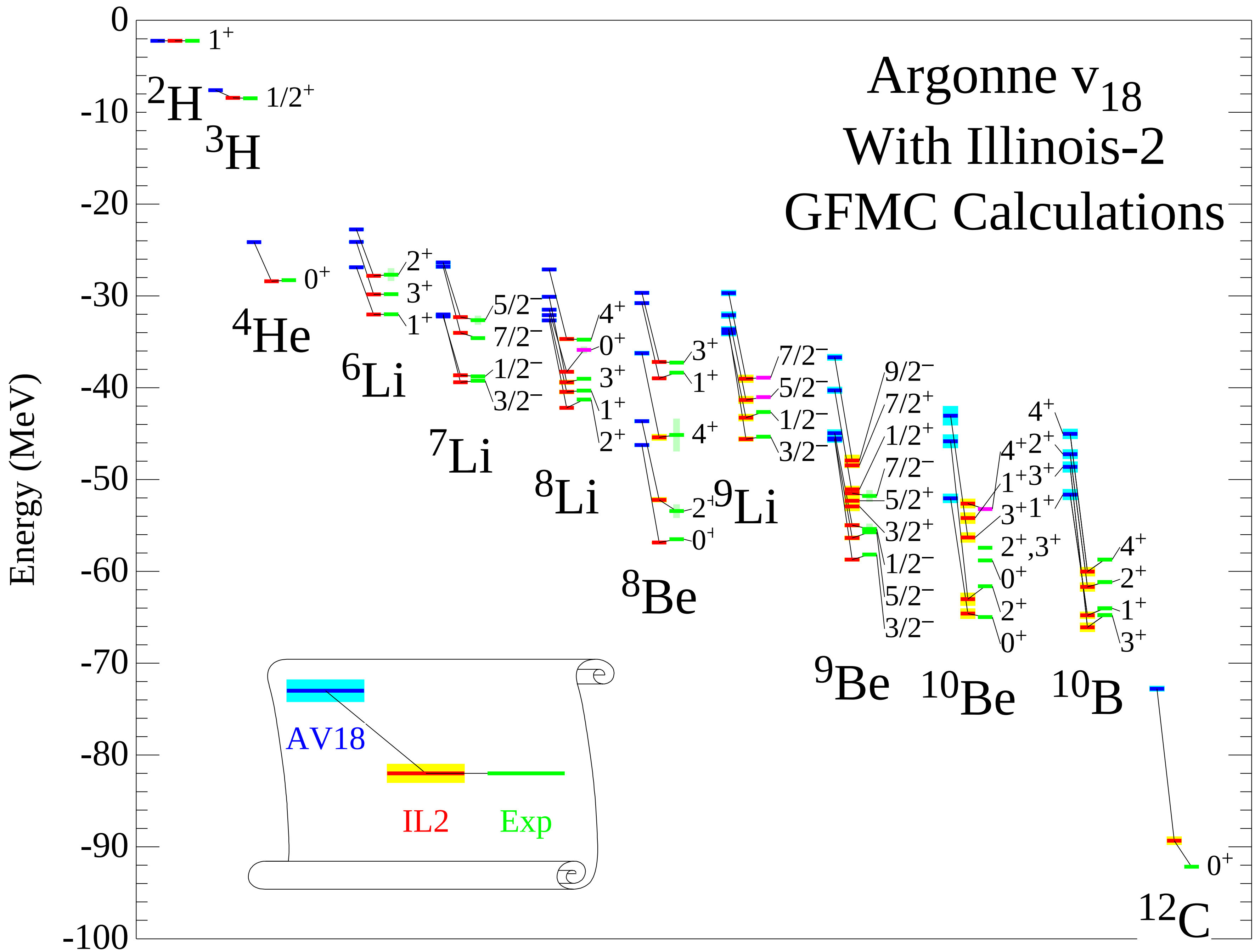
Energy (MeV)
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
4He
0+
6Li
2+
3+
α+d
1+
7Li
5/2−
7/2−
α+t
1/2−
3/2−
8Be
3+
1+
4+
2+
2α
0+
9Be
9/2−
7/2−
1/2−
5/2−
2α+n
3/2−
10Be
4+
1+
3+
9Be+n
2+
0+
10B
4+
6Li+α
2+
1+
3+
ΨT
GFMC
Argonne v18 + IL2
VMC Trial &
GFMC Calculations



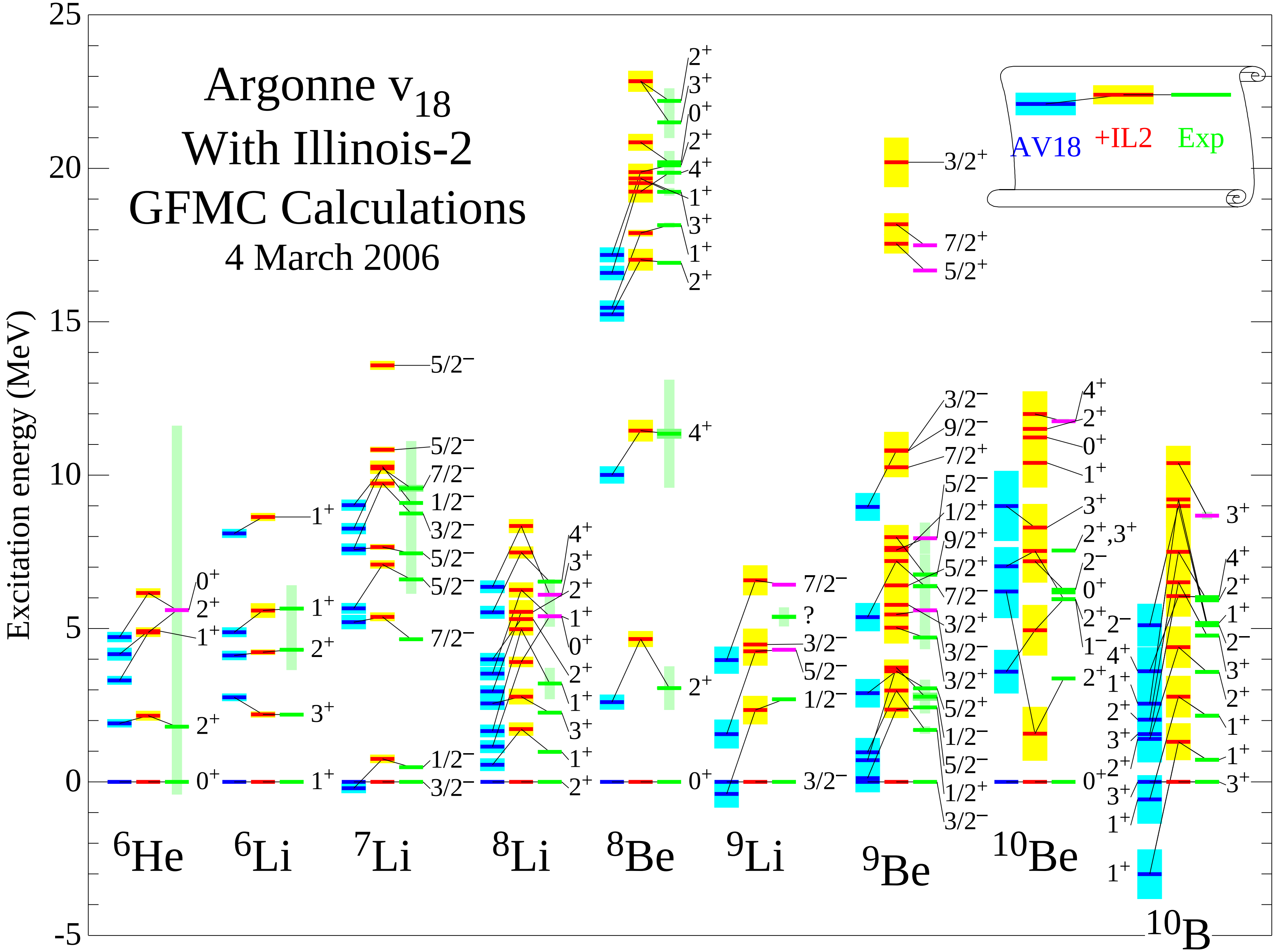
Energy (MeV)
-20
-25
-30
-35
-40
-45
-50
-55
-60
4He
6He
6Li
7Li
8He
8Li
8Be
0+
1+
2+
0+
α+2n
1+
2+
3+
α+d
1+
5/2−
5/2−
7/2−
3/2−
5/2−
5/2−
7/2−
α+t
1/2−
3/2−
1+
2+
6He+2n
0+
4+
0+
1+
3+
7Li+n
1+
2+
3+
1+
2+
4+
2+
0+
2α
AV18
UIX
IL2
Exp
Argonne v18
without & with various Vijk
GFMC Calculations



Argonne v_{18}
without & with V_{ijk}
GFMC Calculations
AV18
UIX
IL2
Exp
Energy (MeV)
-30
-35
-40
-45
-50
-55
-60
-65
7/2⁻
?
5/2⁻
3/2⁻
^{8}Li+n
1/2⁻
3/2⁻
^{9}Li
1/2⁻
5/2⁻
2α+n
3/2⁻
^{9}Be
3,2⁺
^{9}Be+n
0⁺
2⁺
0⁺
^{10}Be
3⁺
1⁺
^{6}Li+α
1⁺
3⁺
^{10}B



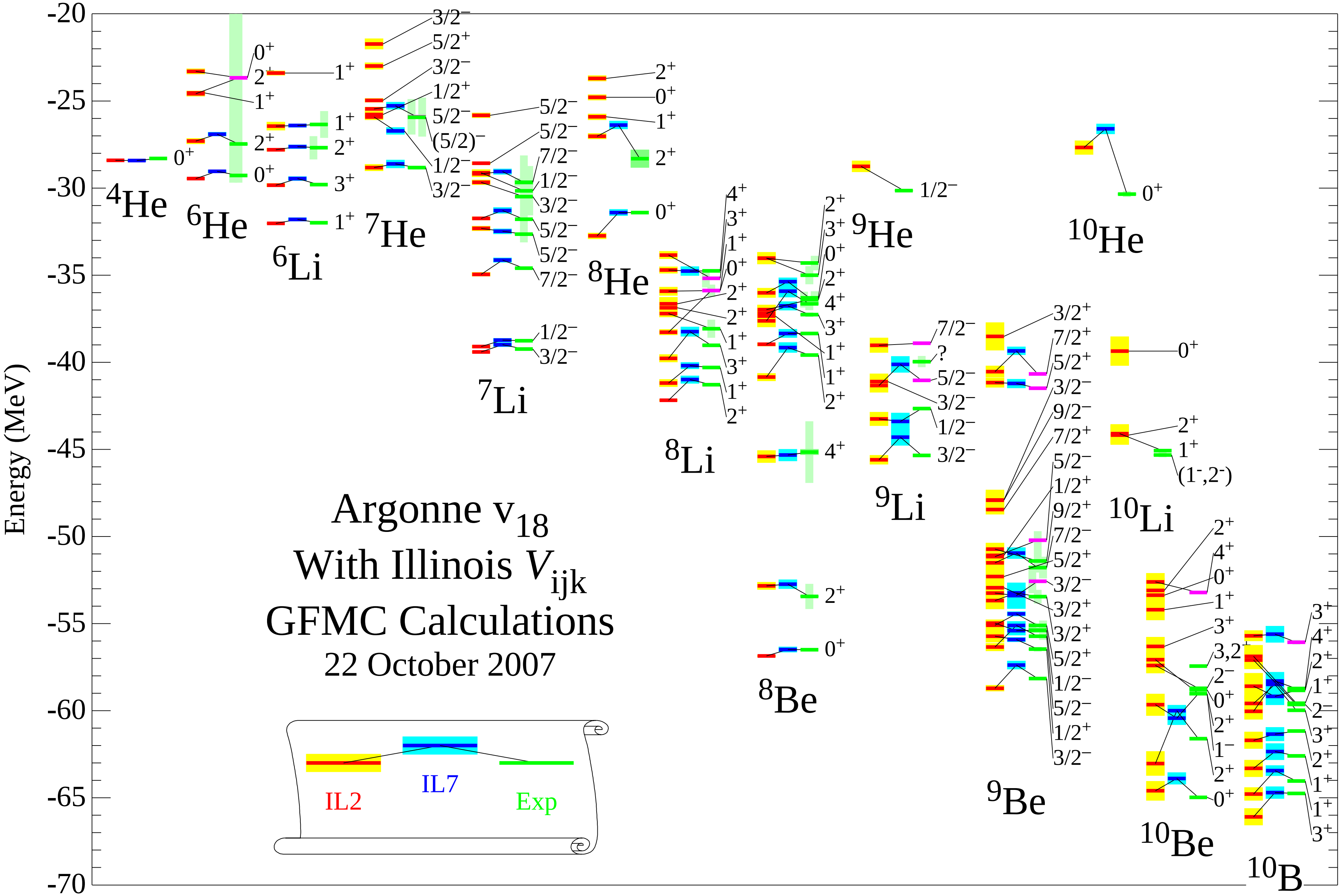
Argonne v18
With Illinois-2
GFMC Calculations
Energy (MeV)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
2H
3H
4He
6Li
7Li
8Li
8Be
9Li
9Be
10Be
10B
12C
AV18
IL2
Exp



Argonne v18
With Illinois-2
GFMC Calculations
4 March 2006
AV18
+IL2
Exp
Excitation energy (MeV)
6He
6Li
7Li
8Li
8Be
9Li
9Be
10Be
10B

NEW ILLINOIS POTENTIALS – PROGRESS REPORT I

- Illinois 1–5 parameters determined in 2000.
  - Fits made to $A \leq 8$ only
  - Preliminary nuclear matter calculations at Urbana (Morales, Pandharipande, Ravenhall) suggested at most IL2 is viable
  - Improved GFMC results in worse ^{8}He agreement
- Started new fitting up to $A = 10$
- Michele Viviani (Pisa) finds sign error in one piece of A_σ in $V_{ijk}^{3\pi}$
  – Formula was published correctly, but incorrectly programmed
  – Increased attraction for all nuclei
- New fit made with corrected A_σ: IL7
  - parameters weaker than for IL2 because of increased attraction
  - better quality reproduction of energies than IL2
  - so far have not found any significant difference in other observables
- Nuclear and neutron matter are probably still too soft



Argonne v18
With Illinois Vijk
GFMC Calculations
22 October 2007
Energy (MeV)
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
4He
6He
6Li
7He
7Li
8He
8Li
8Be
9He
9Li
9Be
10He
10Li
10Be
10B
IL2
IL7
Exp

GFMC FOR SCATTERING STATES

GFMC treats nuclei as particle-stable system – should be good for energies of narrow resonances

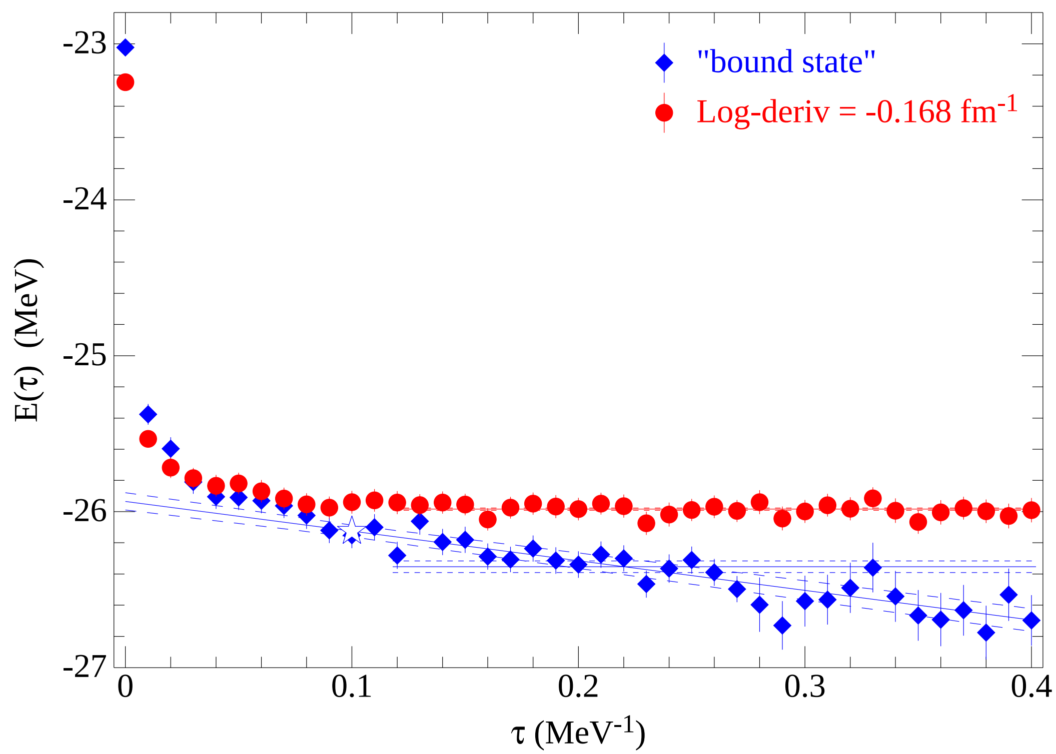
Need better treatment for locations and widths of wide states and for capture reactions

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

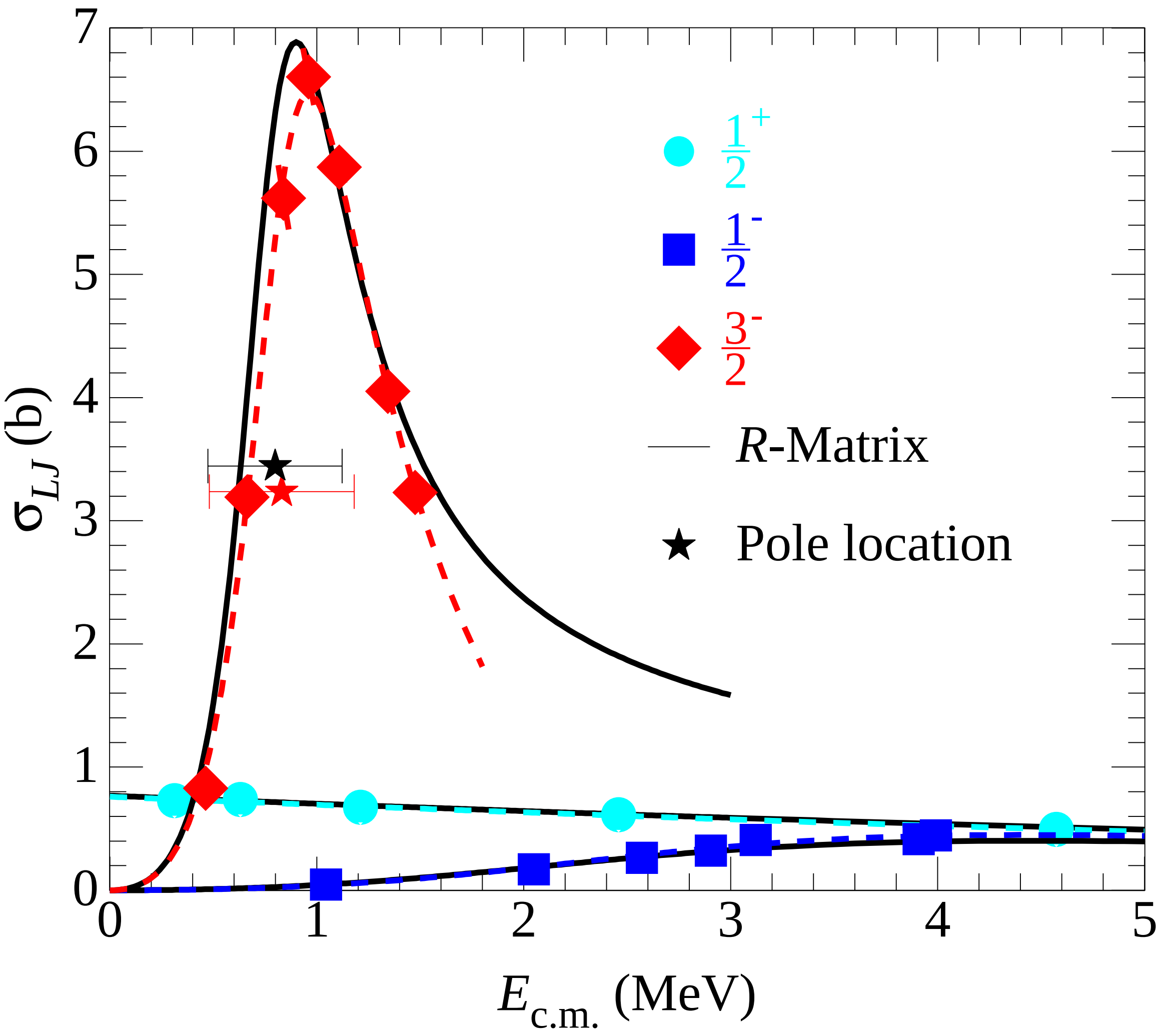
Example for ^{5}He($\frac{1}{2}^-$)

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



^{4}He + n – PARTIAL-WAVE CROSS SECTIONS

- Hale phase shifts from R-matrix analysis up to $J = \frac{9}{2}$ of data
- Tilted error bars from $\delta(R_B, \chi, E \pm \Delta E)$
- AV18+IL2 was not fit to ^{5}He, good prediction of $\frac{3}{2}^-$ & $\frac{1}{2}^-$ resonances (both locations and widths)
- ^{4}He+n scattering length also well reproduced



Nollett, *et al.*, Phys.Rev.Lett. **99**, 022502 (2007)

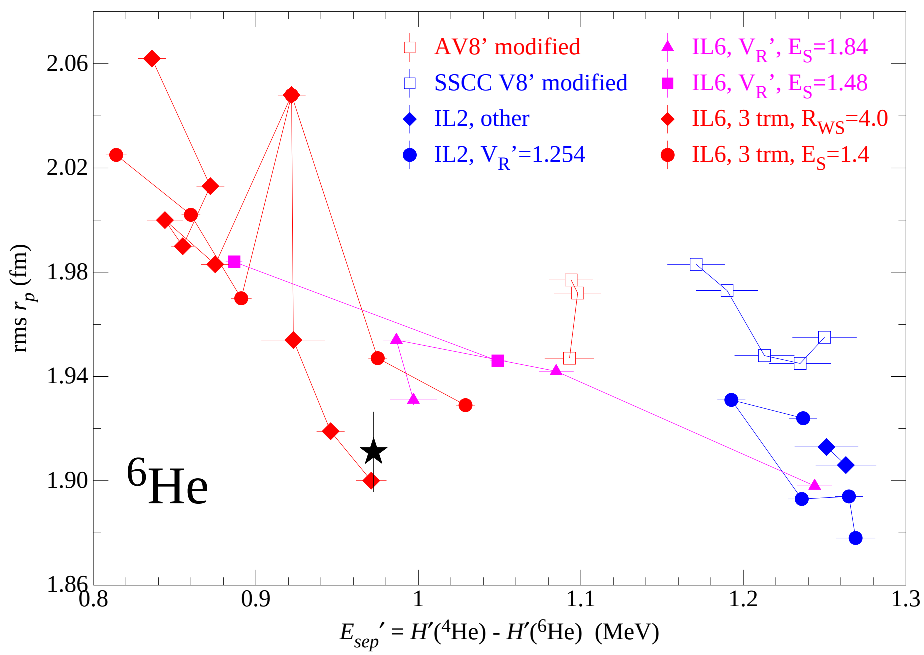
RMS Radii of Helium Isotopes

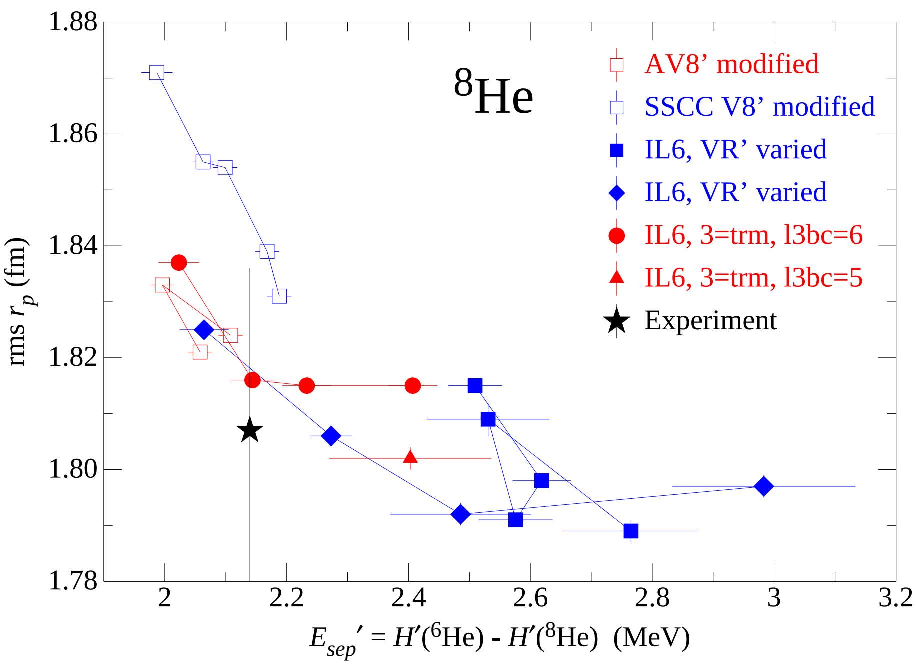
Recent measurement of ^{6}He charge radius at Argonne and ^{8}He at GANIL

- Single ^{4}He or ^{6}He or ^{8}He atoms trapped
- Isotope shift of an atomic transition measured
- Small $\langle r^2 \rangle^{1/2}$ dependence of shift extracted using precise atomic calculations
- ^{6}He half-life only 0.807s; ^{8}He half-life only 0.119s

GFMC radius strongly dependent on propagated separation energy

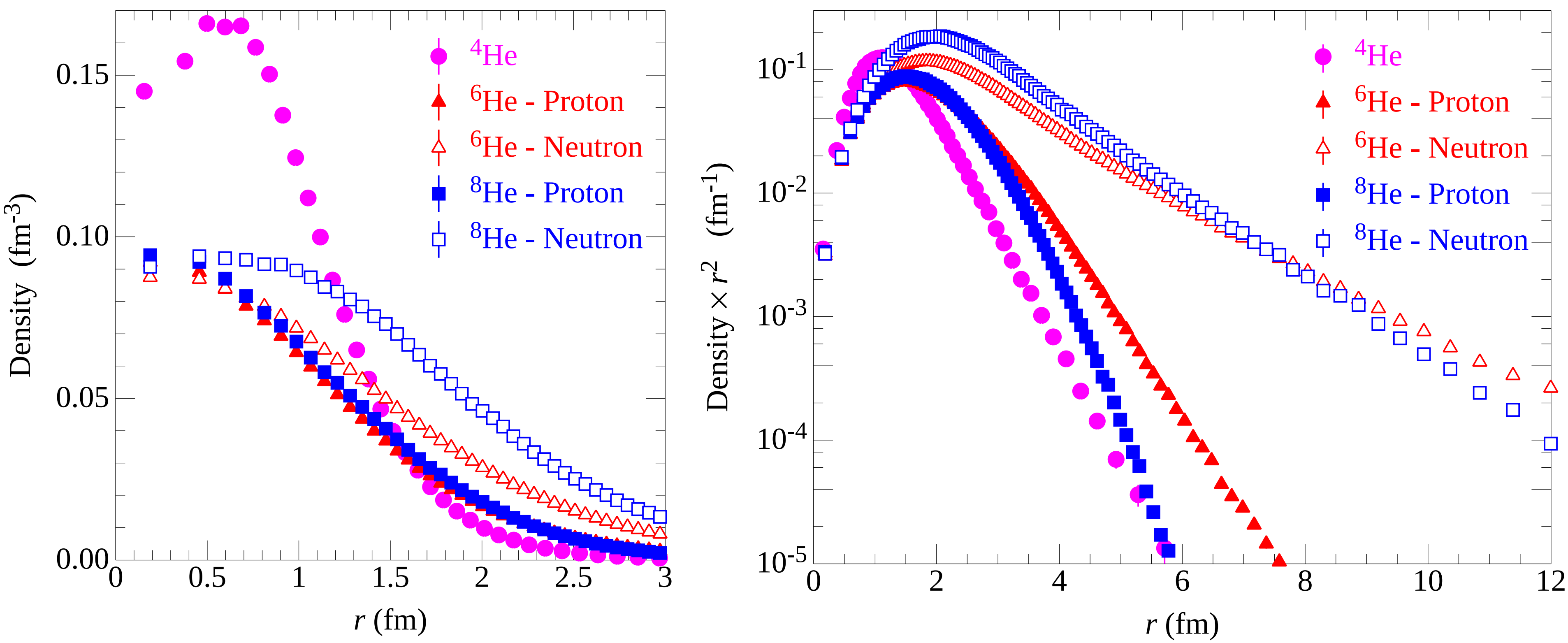
^{8}He charge radius smaller than for ^{6}He





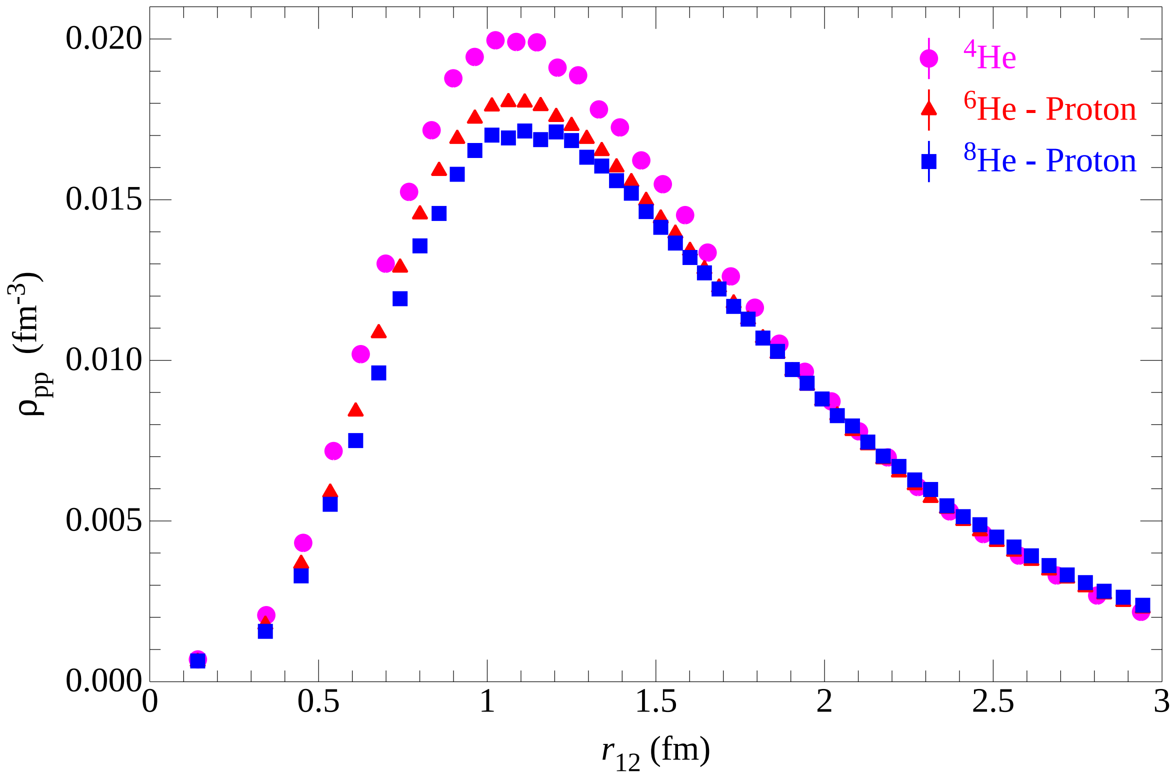
^{4,6,8}He Densities

- ^{4}He central density twice that of nuclear matter!
- Neutrons drag ^{4}He center of mass around – spread out density
  – results in charge radius of ^{6}He $>$ ^{4}He (2.08 fm vs 1.66 fm)
- ^{6}He & ^{8}He have large neutron halos due to weak binding of neutrons
- Neutron halo of ^{6}He more diffuse than that of ^{8}He – smaller E_{sep}



Two-nucleon densities

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

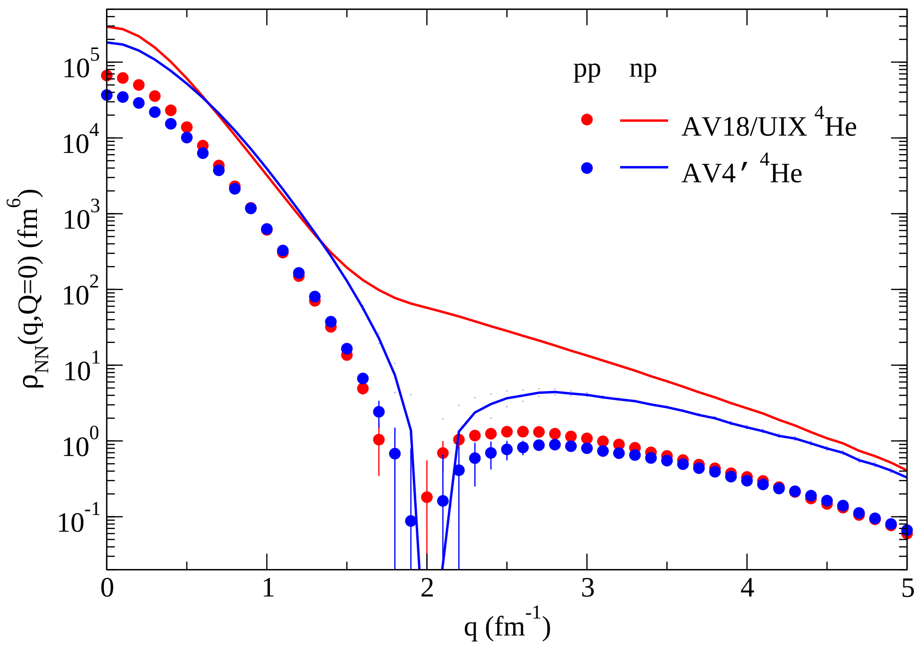


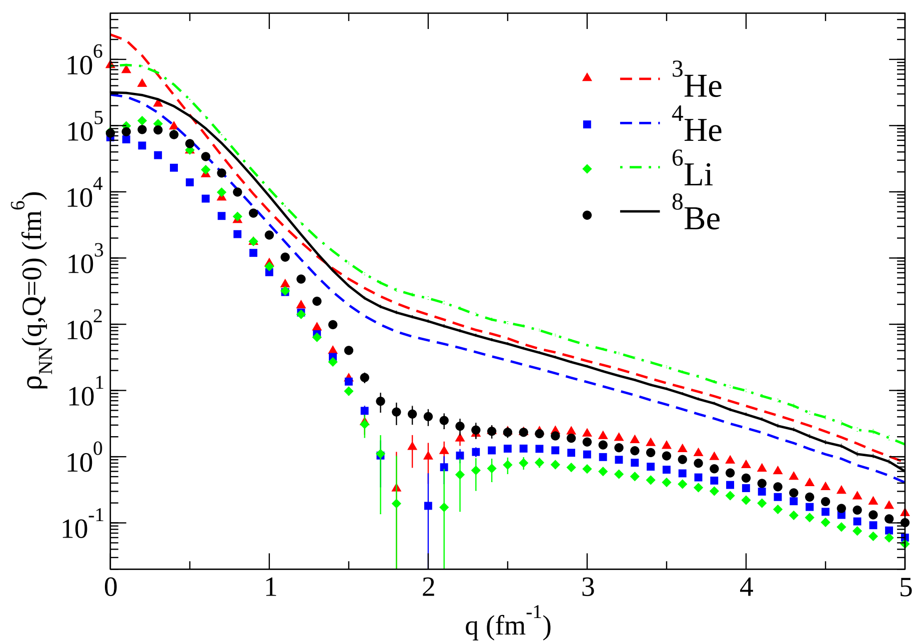
pair rms radii

	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 KNOCKOUT – $(e, e'pN)$

- Recent (still being analyzed) JLab expt. for ^{12}C$(e, e'pN)$
- Measured back to back pp and np pairs
- Pairs with relative momentum 2–3 fm^{-1} show 10–20 $\times$ np enhancement (preliminary).





- VMC calculations for ^{3}He, ^{4}He, and ^{8}Be show this effect
- Effect disappears when tensor correlations are turned off
- Shows importance of tensor correlations to > 2 fm^{-1}.

GFMC FOR OFF-DIAGONAL MATRIX ELEMENTS

We can generalize the "mixed" estimates of expectation values for off-diagonal matrix elements

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

where

$$\begin{aligned}
\langle O\rangle_V &= \frac{\langle \Psi^f_T|O|\Psi^i_T\rangle}{\sqrt{\langle \Psi^f_T|\Psi^f_T\rangle}\sqrt{\langle \Psi^i_T|\Psi^i_T\rangle}} \ , \\
\langle O(\tau)\rangle_{M_i} &= \frac{\langle \Psi^f_T|O|\Psi^i(\tau)\rangle}{\langle \Psi^i_T|\Psi^i(\tau)\rangle}\sqrt{\frac{\langle \Psi^i_T|\Psi^i_T\rangle}{\langle \Psi^f_T|\Psi^f_T\rangle}} \ , \\
\langle O(\tau)\rangle_{M_f} &= \frac{\langle \Psi^f(\tau)|O|\Psi^i_T\rangle}{\langle \Psi^f(\tau)|\Psi^f_T\rangle}\sqrt{\frac{\langle \Psi^f_T|\Psi^f_T\rangle}{\langle \Psi^i_T|\Psi^i_T\rangle}} \ ,
\end{aligned}$$

Electromagnetic Transitions of $A = 6, 7$ Nuclei – Widths in eV

$J_i^P \rightarrow J_f^P$	Transition	VMC	GFMC	Expt
$^6\mathrm{Li}(3^+) \rightarrow {}^6\mathrm{Li}(1^+)$	$E2\ (10^{-4})$	3.86	4.68(5)	4.40(34)
$^6\mathrm{Li}(0^+) \rightarrow {}^6\mathrm{Li}(1^+)$	$M1\ (10^{0})$	7.10	6.86(2)	8.19(17)
$^7\mathrm{Li}(\frac{1}{2}^-) \rightarrow {}^7\mathrm{Li}(\frac{3}{2}^-)$	$E2\ (10^{-7})$	2.61	3.24(7)	3.30(20)
$^7\mathrm{Li}(\frac{1}{2}^-) \rightarrow {}^7\mathrm{Li}(\frac{3}{2}^-)$	$M1\ (10^{-3})$	4.74	4.58(3)	6.30(31)
$^7\mathrm{Li}(\frac{7}{2}^-) \rightarrow {}^7\mathrm{Li}(\frac{3}{2}^-)$	$E2\ (10^{-2})$	1.29	1.74(2)	1.50(20)
$^7\mathrm{Be}(\frac{1}{2}^-) \rightarrow {}^7\mathrm{Be}(\frac{3}{2}^-)$	$E2\ (10^{-7})$	4.24	6.00(7)	—
$^7\mathrm{Be}(\frac{1}{2}^-) \rightarrow {}^7\mathrm{Be}(\frac{3}{2}^-)$	$M1\ (10^{-3})$	2.69	2.62(1)	3.43(45)

Weak Transitions of $A = 6, 7$ Nuclei – log(ft)

$J_i^P \rightarrow J_f^P$	Transition	VMC	GFMC	Expt
$^6\mathrm{He}(0^+) \rightarrow {}^6\mathrm{Li}(1^+)$	GT	2.901	2.916	2.910
$^7\mathrm{Be}(\frac{3}{2}^-) \rightarrow {}^7\mathrm{Li}(\frac{3}{2}^-)$	F & GT	3.288	3.302	3.32
$^7\mathrm{Be}(\frac{3}{2}^-) \rightarrow {}^7\mathrm{Li}(\frac{1}{2}^-)$	GT	3.523	3.542	3.55
$^7\mathrm{Li}(\frac{1}{2}^-)\ /\ {}^7\mathrm{Li}(\frac{3}{2}^-)$	F & GT	10.38%	10.25%	10.44%

Isospin-mixing in ^{8}Be

Experimental energies of 2^+ states

E_a = 16.626(3) MeV

E_b = 16.922(3) MeV

and 2α decay widths:

Γ_a = 108.1(5) keV

Γ_b = 74.0(4) keV

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

$\Psi_a = \alpha\Psi_0 + \beta\Psi_1$

$\Psi_b = \beta\Psi_0 - \alpha\Psi_1$

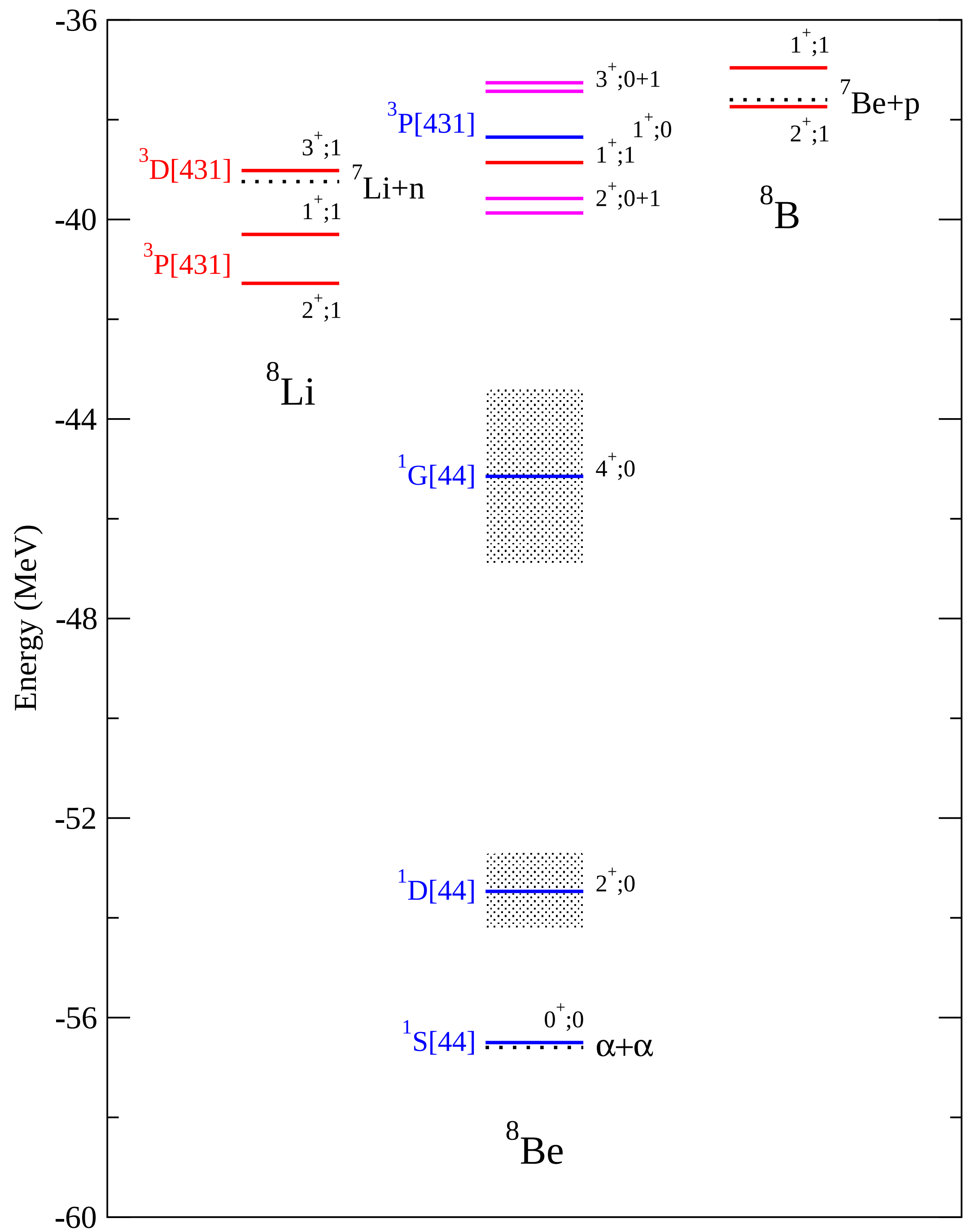
$\alpha^2 + \beta^2 = 1$

Decay through $T = 0$ component only

$\Gamma_a/\Gamma_b = \alpha^2/\beta^2$

$\alpha = 0.7705(15)$

$\beta = 0.6375(19)$



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

$$H_{00} = 16.746(2)\ \mathrm{MeV}$$
$$H_{11} = 16.802(2)\ \mathrm{MeV}$$
$$H_{01} = -145(3)\ \mathrm{keV}$$

F. C. Barker [Nucl.Phys. **83**, 418 (1966)] estimated the Coulomb matrix element connecting the 2^+;1 and 2^+;0* states as $H_{01}^{\mathrm{C}} = -67$ keV

The 1^+;1 and 1^+;0 and the 3^+;1 and 3^+;0 levels also mix, but decay by nucleon emission. Barker assigns values of:

$$\alpha_1 = 0.24\ ;\ \beta_1 = 0.97\ ;\ H_{01} = -120(1)\ \mathrm{keV}$$
$$\alpha_3 = 0.41\ ;\ \beta_3 = 0.91\ ;\ H_{01} = -62(15)\ \mathrm{keV}$$

Isospin-mixing matrix elements in keV

		H_{01}	K^{CSB}	V^{CSB}	V_γ	(Coul)	(Mag)
$2^+;1 \Leftrightarrow 2^+;0$*	VMC	$-107(2)$	$-2.5(2)$	$-23.8(4)$	$-80.8(12)$	$-69.4(11)$	$-11.4(1)$
	GFMC	$-115(3)$	$-3.1(2)$	$-21.3(6)$	$-90.3(26)$	$-78.3(25)$	$-12.0(2)$
	Barker	$-145(3)$				-67	
$1^+;1 \Leftrightarrow 1^+;0$	VMC	$-70(1)$	$-1.8(1)$	$-17.5(3)$	$-50.4(9)$	$-50.6(9)$	$0.2(1)$
	GFMC	$-102(4)$	$-2.9(2)$	$-18.2(6)$	$-80.3(30)$	$-79.5(30)$	$-0.8(2)$
	Barker	$-120(1)$				-54	
$3^+;1 \Leftrightarrow 3^+;0$	VMC	$-67(1)$	$-1.4(1)$	$-12.7(3)$	$-52.0(6)$	$-41.0(6)$	$-12.0(2)$
	GFMC	$-90(3)$	$-2.5(2)$	$-14.8(6)$	$-73.1(21)$	$-60.9(21)$	$-12.2(2)$
	Barker	$-62(15)$				-32	
$2^+;1 \Leftrightarrow 2^+;0$	VMC	$-13(1)$	$-0.2(1)$	$-2.4(1)$	$-10.4(3)$	$-6.1(2)$	$-4.3(1)$
	GFMC	$-6(2)$	$-0.4(2)$	$-1.3(4)$	$-4.4(12)$		

CONCLUSIONS

We have made much progress in calculating light nuclei

- $1-2\%$ calculations of A = 6 – 12 nuclear energies are possible
- Illinois V_{ijk} give average binding-energy errors < 0.7 MeV for $A = 3-12$
  - – V_{ijk} required for overall P-shell energies
  - – Also required for spin-orbit splittings and several level orderings
- Charge radii are in good agreement with experiment
- GFMC for off-diagonal matrix elements in progress
- GFMC for scattering states has been initiated
- VMC calculations of single- and multi-nucleon momentum distributions

and there is still much to do

- Lots of scattering states and reactions to be done
  - n+^{3}H, p+α, n+^{6}He, n+^{8}He, n+^{9}Li, α+α, *etc.*
  - astrophysical reactions: ^{3}He+$\alpha \rightarrow ^7$Be, p+^{7}Be $\rightarrow ^8$B, n+(α+α) $\rightarrow ^9$Be, *etc.*
    - – All big-bang nucleosynthesis, solar, & some r-process seeding reactions should be accessible
- Calculations of
  - overlaps, spectroscopic factors, asymptotic normalization coefficients
  - electromagnetic and weak transitions in $A \geq 8$ nuclei
  - meson-exchange current contributions to moments and transitions
  - more unnatural-parity & $2\hbar\omega$ excited states
- ^{12}C including 2nd 0$^+$ (Hoyle) state