Quantum Monte Carlo and double-beta decay

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Physics Division

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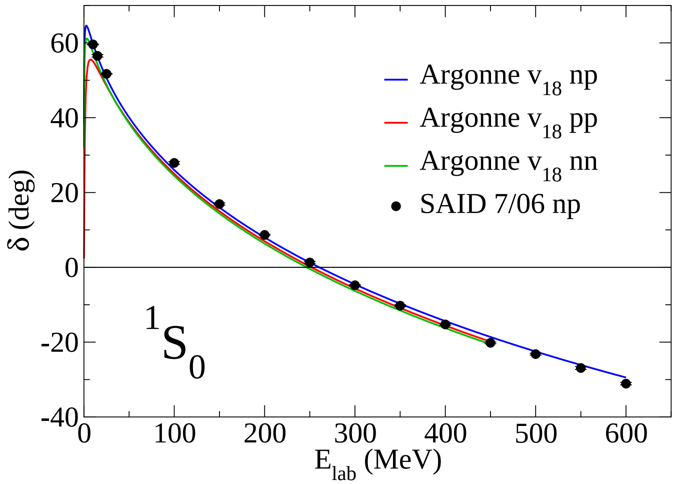
NUCLEAR HAMILTONIAN

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

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

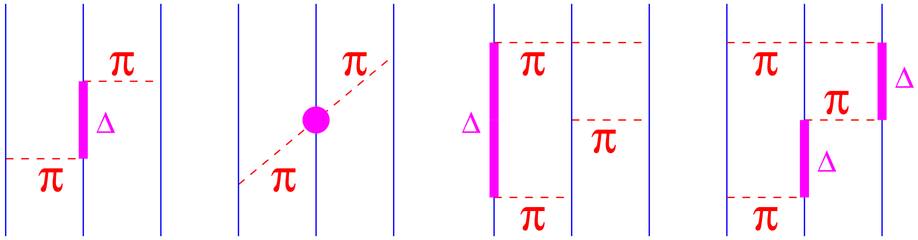
Argonne v$_{18}$: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij}) O_{ij}^p$

- 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 χ^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 2π P-wave + short-range repulsion for matter saturation
- Illinois adds 2π S-wave + 3π 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)

Norfolk v$_{17}$: $v_{ij} = v^{\gamma}_{ij} + v^{\pi}_{ij} + v^{2\pi}_{ij} + v^{C}_{ij} = \sum v_p(r_{ij}) O^p_{ij}$

- derived in chiral effective field theory with Δ-intermediate states
- 17 spin, tensor, spin-orbit, isospin, etc., operators
- full EM and strong CD and CSB terms included
- predominantly local operator structure suitable for quantum Monte Carlo
- multiple models with varying regularization
- fit Granada PWA2013 data to $E_{\rm lab}$ = 125 MeV with χ^2/d.o.f.$\sim$1.1
  (or 200 MeV with χ^2/d.o.f.$\sim$1.4)

Piarulli, Girlanda, Schiavilla, Perez, Armaro, & Arriola PRC **91**, (2015)

Norfolk $V_{ijk} = V^{2\pi}_{ijk} + V^{D}_{ijk} + V^{E}_{ijk}$

- standard 2π S-wave and 2π P-wave terms consistent with NN potential
- short-range contact terms of c_D and c_E type
- two parameters fit to ^{3}H binding and nd scattering length

Piarulli, Baroni, Girlanda, Kievsky, Lovato, Marcucci, Pieper, Schiavilla, Viviani, & Wiringa (in preparation)

QUANTUM MONTE CARLO

Variational Monte Carlo (VMC): construct Ψ_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^π states
- Minimize $E_V = \langle \Psi_V | H | \Psi_V \rangle \geq E$; automated optimization for variational parameters

These are $\sim 2^A \binom{A}{Z}$ component (540,672 for ^{12}C) spin-isospin vectors in $3A$ dimensions

Wiringa, PRC **43**, 1585 (1991)

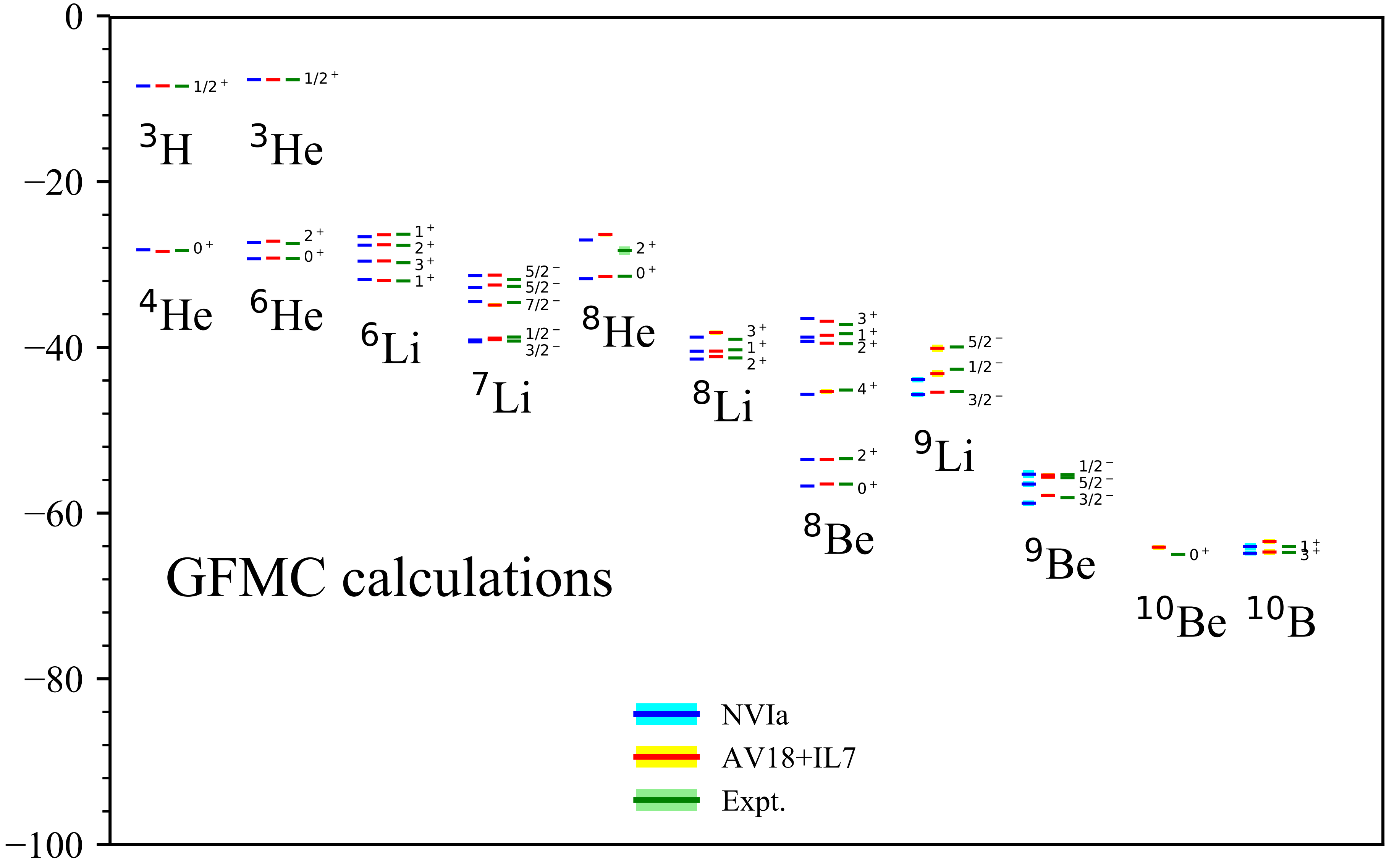
Green's function Monte Carlo (GFMC): project out the exact eigenfunction

- $\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau] a_n \Psi_n \Rightarrow \Psi_0$ at large τ
- Propagation done stochastically in small time slices $\Delta\tau$
- Exact $\langle H \rangle$ for local potentials; mixed estimates for other $\langle O \rangle$
- Constrained-path propagation controls fermion sign problem for $A \geq 8$ ($A \geq 4$ for NV17)
- Multiple excited states for same J^π stay orthogonal

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

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

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


0
−20
−40
−60
−80
−100
GFMC calculations
^{3}H
1/2$^+$
^{3}He
1/2$^+$
^{4}He
0$^+$
^{6}He
2$^+$
0$^+$
^{6}Li
1$^+$
2$^+$
3$^+$
1$^+$
^{7}Li
5/2$^-$
5/2$^-$
7/2$^-$
1/2$^-$
3/2$^-$
^{8}He
2$^+$
0$^+$
^{8}Li
3$^+$
1$^+$
2$^+$
^{8}Be
3$^+$
1$^+$
2$^+$
4$^+$
2$^+$
0$^+$
^{9}Li
5/2$^-$
1/2$^-$
3/2$^-$
^{9}Be
1/2$^-$
5/2$^-$
3/2$^-$
^{10}Be
0$^+$
^{10}B
1$^+$
3$^+$
NVIa
AV18+IL7
Expt.

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

NO EFFECTIVE CHARGES!

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

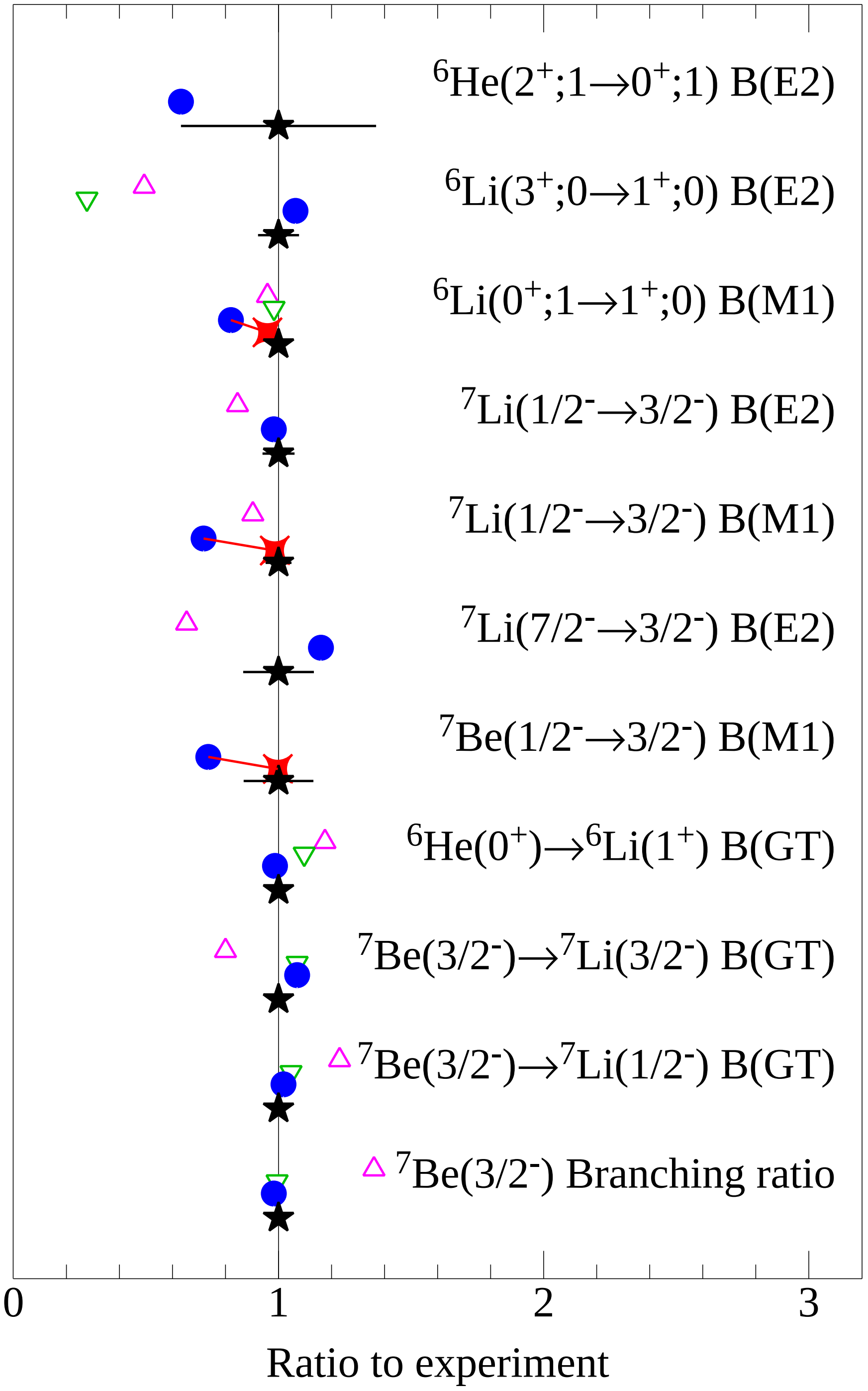
$$M1 = \mu_N \sum_k [(L_k \; + \; g_p S_k)(1 + \tau_{kz})/2 \\ + g_n S_k \;\; (1 - \tau_{kz})/2]$$

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

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

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

- △ Cohen-Kurath
- ▽ NCSM
- ● GFMC(IA)
- ✦ GFMC(MEC)
- ★ Experiment

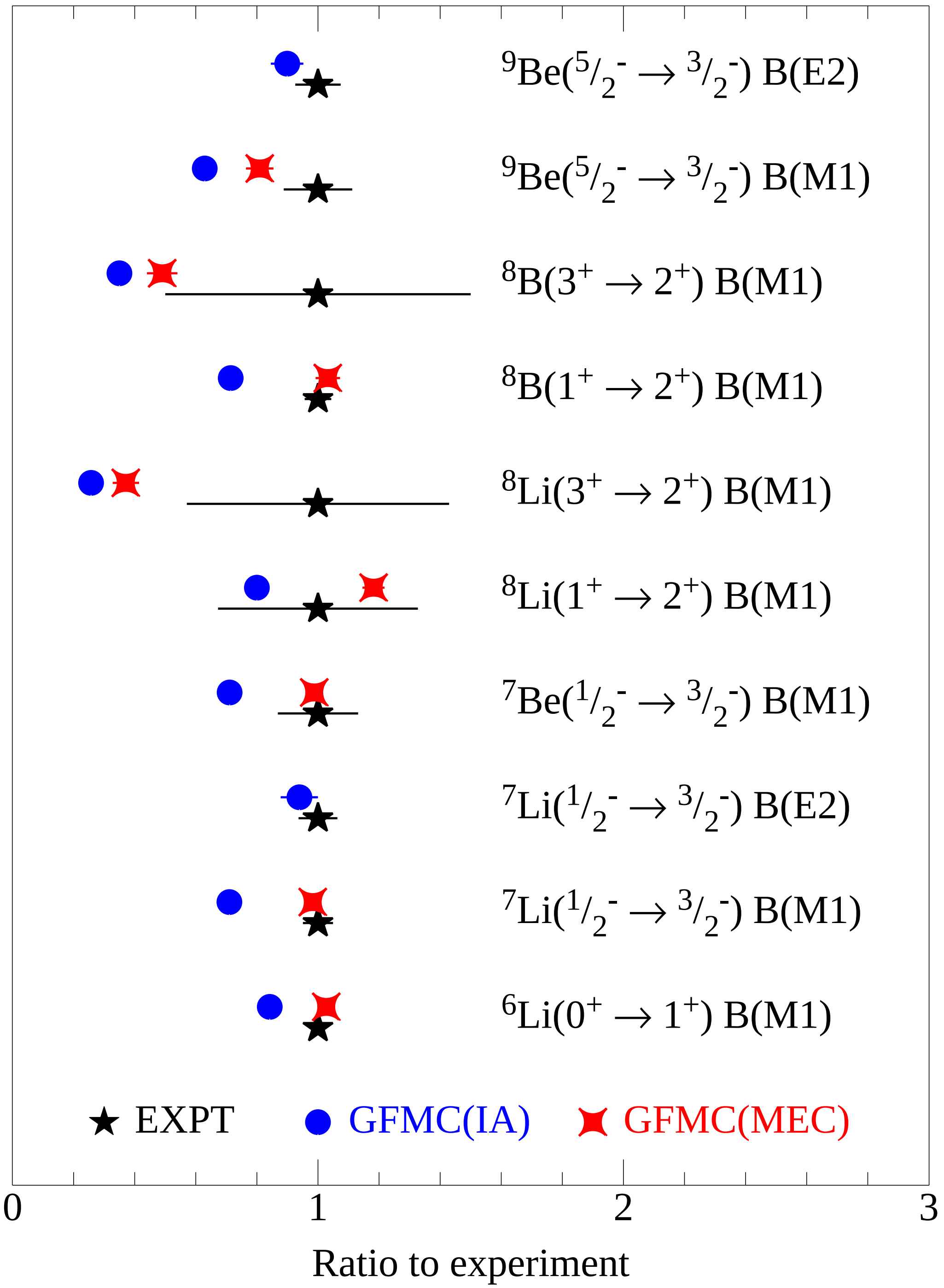


$M1$ TRANSITIONS W/ χEFT

- 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)



VMC-IA Electroweak Transition Survey

VMC IA comparison				NV17-106	AV18+UX
6Li	2.19 -> 0	3+ -> 1+	E2	8.00 (5)	8.10 (5)
	3.56 -> 0	0+;1 -> 1+;0	M1	3.737 (2)	3.664 (5)
	4.31 -> 0	2+ -> 1+	E2	6.07 (5)	6.10 (4)
	5.37 -> 0	2+;1 -> 1+;0	M1	0.252 (3)	0.280 (8)
7Li	0.48 -> 0	1/2- -> 3/2-	M1	2.790 (6)	2.769 (6)
			E2	4.85 (4)	4.47 (3)
	4.65 -> 0	7/2- -> 3/2-	E2	7.15 (4)	6.79 (3)
7Be	0.43 -> 0	1/2- -> 3/2-	M1	2.447 (2)	2.429 (2)
8Li	0.98 -> 0	1+ -> 2+	M1	3.315 (3)	3.628 (3)
	2.26 -> 0	3+ -> 2+	M1	1.123 (3)	1.095 (3)
8Be	3.03 -> 0	2+ -> 0+	E2	8.77 (6)	8.74 (5)
	11.4 -> 3.03	4+ -> 2+	E2	11.59 (6)	13.04 (6)
	16.6 -> 0	2+ -> 0+	E2	0.229 (5)	0.113 (4)
	-> 3.03	2+ -> 2+	M1	0.0290 (6)	0.0145 (6)
	16.9 -> 0	2+;1 -> 0+	E2	0.423 (3)	0.326 (2)
	-> 3.03	2+;1 -> 2+	M1	0.453 (3)	0.307 (2)
	17.6 -> 0	1+;1 -> 0+	M1	0.653 (2)	0.571 (2)
	-> 3.03	1+;1 -> 2+	M1	0.480 (2)	0.426 (1)
	-> 16.6	1+;1 -> 2+	M1	2.488 (5)	2.453 (9)
	-> 16.9	1+;1 -> 2+;1	M1	0.181 (3)	0.172 (2)
	18.1 -> 0	1+ -> 0+	M1	0.0162 (1)	0.0115 (1)
	-> 3.03	1+ -> 2+	M1	0.020 (2)	0.0098 (2)
	-> 16.6	1+ -> 2+	M1	0.188 (4)	0.217 (3)
	-> 16.9	1+ -> 2+;1	M1	2.37 (1)	2.72 (1)

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10Be 3.37 -> 0       2+  -> 0+     E2    6.22 (5)     6.40 (5)
     5.96 -> 0       2+  -> 0+     E2    1.45 (3)     0.32 (5)

10B  0.72 -> 0       1+  -> 3+     E2    3.10 (4)     3.58 (3)
     1.74 -> 0.72   0+;1 -> 1+     M1    3.354 (3)    3.523 (3)
     2.15 -> 0       1+  -> 3+     E2    0.88 (1)     0.57 (1)
          -> 0.72    1+  -> 1+     M1    0.036 (3)    0.057(2)
                                   E2    3.58 (6)     2.88 (5)
          -> 1.74    1+  -> 0+;1   M1    0.98 (1)     1.05 (2)
     3.59 -> 0       2+  -> 3+     M1    0.013 (6)    0.056 (2)
                                   E2    1.99 (5)     3.02 (5)
     5.16 -> 1.74   2+;1 -> 0+;1   E2    5.91 (5)     5.58 (6)

10C  3.35 -> 0       2+  -> 0+     E2    5.44 (9)     4.84 (7)

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6He -> 6Li   0+;1 -> 1+;0          GT    2.188 (2)    2.177 (2)

7Be -> 7Li   3/2- -> 3/2-           F    1.9997       1.9998
                                   GT    2.317 (1)    2.335 (1)

7Be -> 7Li*  3/2- -> 1/2-          GT    2.158 (3)    2.150 (1)

8He -> 8Li*  0+;1 -> 1+;1          GT    0.387 (3)    0.340 (1)

8Li -> 8Be*  2+;1 -> 2+;0          GT    0.147 (1)    0.082 (1)

8B  -> 8Be*  2+;1 -> 2+;0          GT    0.146 (1)    0.081 (1)

10C -> 10B   0+;1 -> 1+;0          GT    1.942 (2)    2.062 (3)
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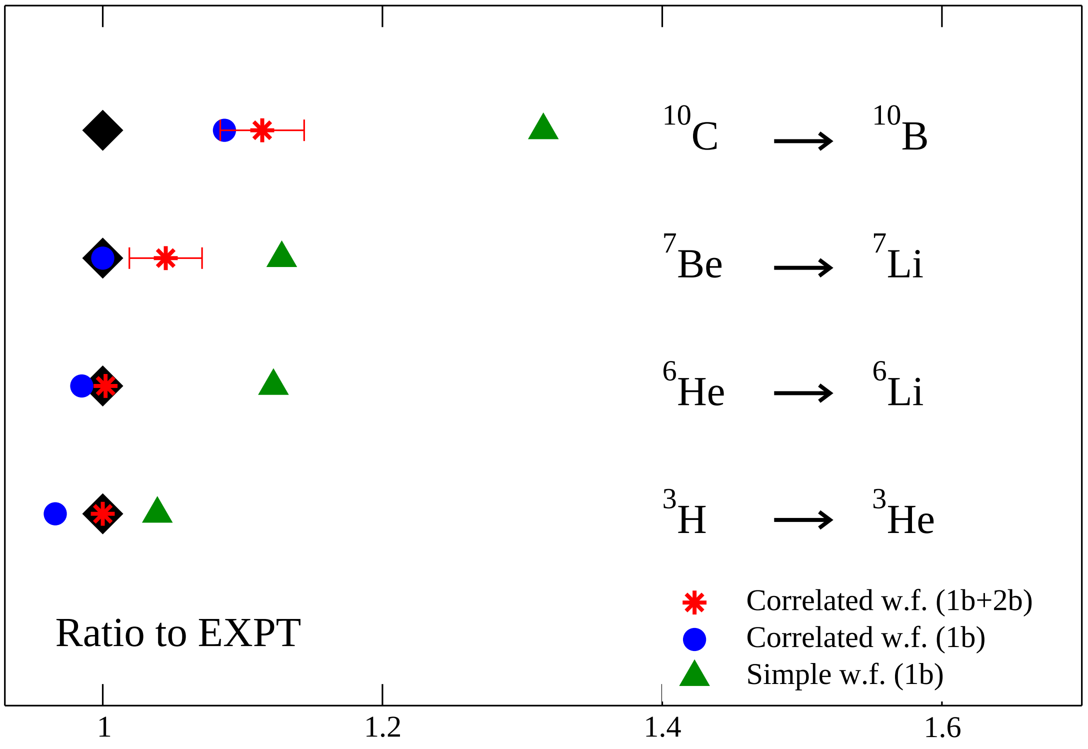
SINGLE β-DECAY



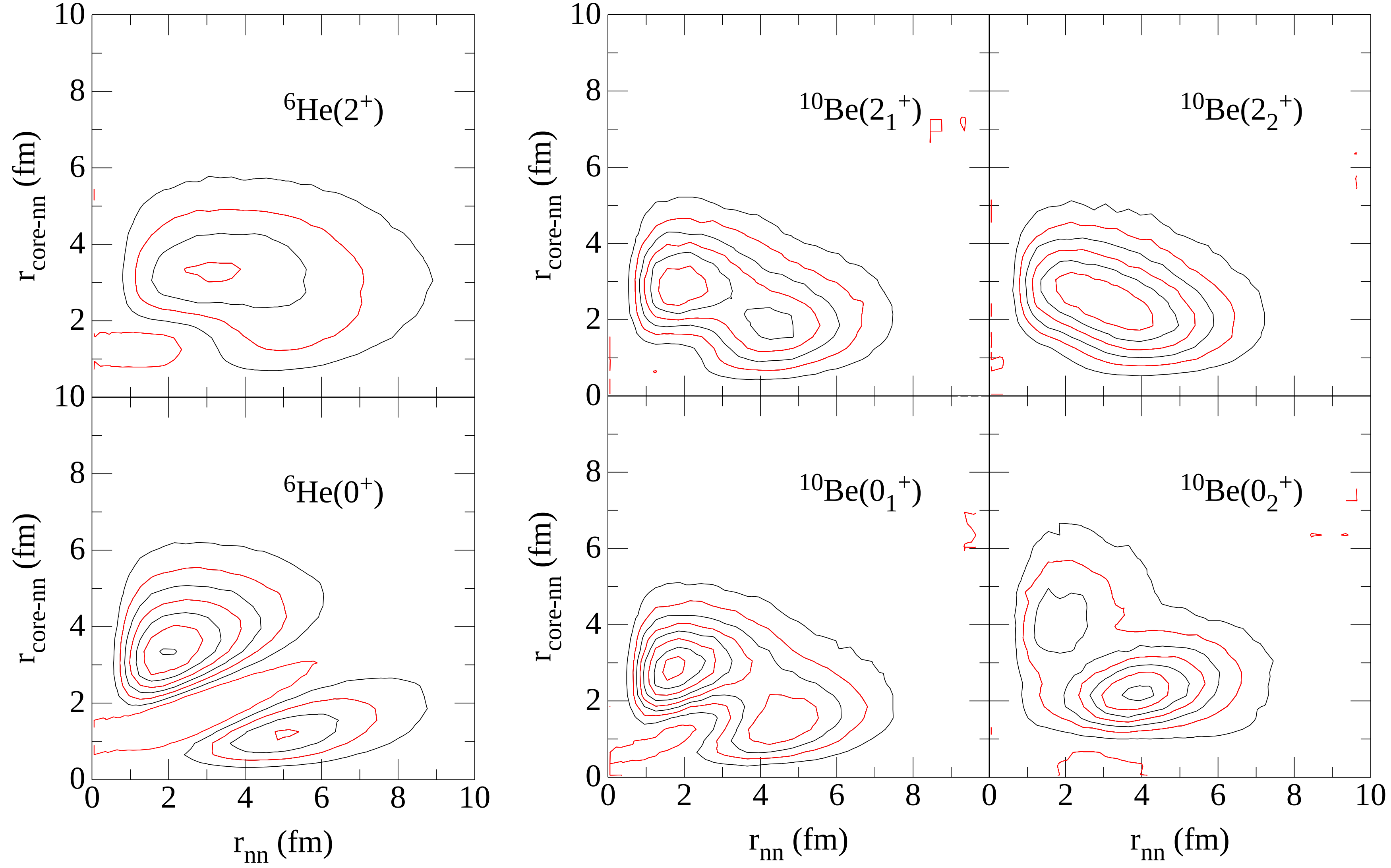
Pastore, Baroni, Carlson, Gandolfi, Pieper, Schiavilla & Wiringa (in preparation)

ORIGIN OF QUENCHING IN QMC WAVE FUNCTIONS

Wave function %	S=0	S=1	S=2	S=3
$^{6}\mathrm{He}(0^{+};1)\vert\Psi_{J}\rangle$	1.0	0.0	0.0	0.0
$^{6}\mathrm{He}(0^{+};1)\vert\Psi_{V}\rangle$	0.76	0.08	0.16	0.005
$^{6}\mathrm{Li}(1^{+};0)\vert\Psi_{J}\rangle$	0.0	1.0	0.0	0.0
$^{6}\mathrm{Li}(1^{+};0)\vert\Psi_{V}\rangle$	0.02	0.86	0.06	0.06
Wave function %	**S=1/2**	**S=3/2**	**S=5/2**	**S=7/2**
$^{7}\mathrm{Be}(3/2^{-};1/2)\vert\Psi_{J}\rangle$	1.0	0.0	0.0	0.0
$^{7}\mathrm{Be}(3/2^{-};1/2)\vert\Psi_{V}\rangle$	0.76	0.15	0.09	0.005
$^{7}\mathrm{Li}(3/2^{-};1/2)\vert\Psi_{J}\rangle$	1.0	0.0	0.0	0.0
$^{7}\mathrm{Li}(3/2^{-};1/2)\vert\Psi_{V}\rangle$	0.76	0.15	0.09	0.005

TWO-NUCLEON HALO DENSITIES

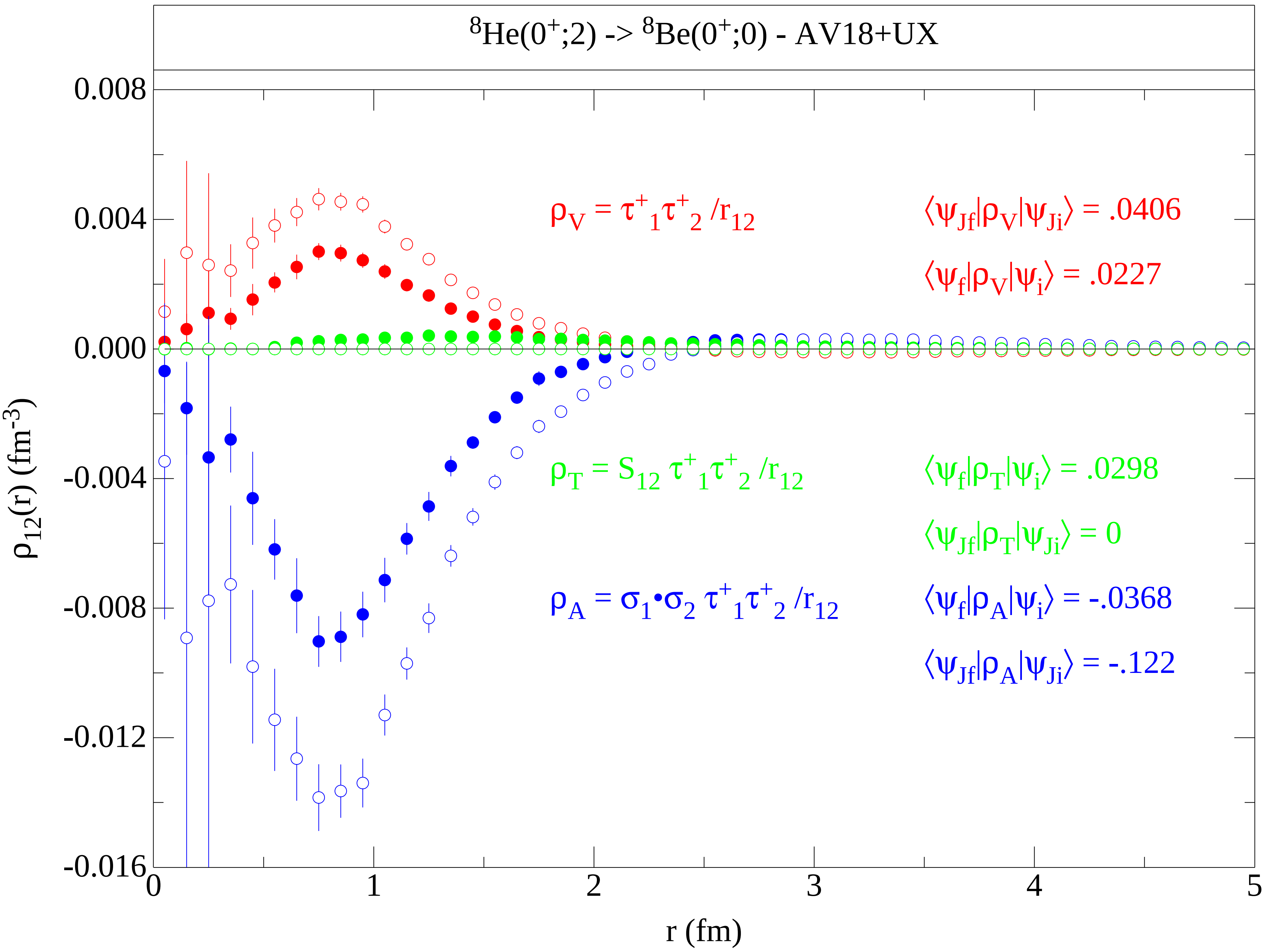
$$\rho_{nn}(r) = \sum_{i<j} \langle \Psi(J^\pi, T, T_z = +1) | \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \tau_i^+ \tau_j^+ | \Psi(J^\pi, T, T_z = -1) \rangle$$



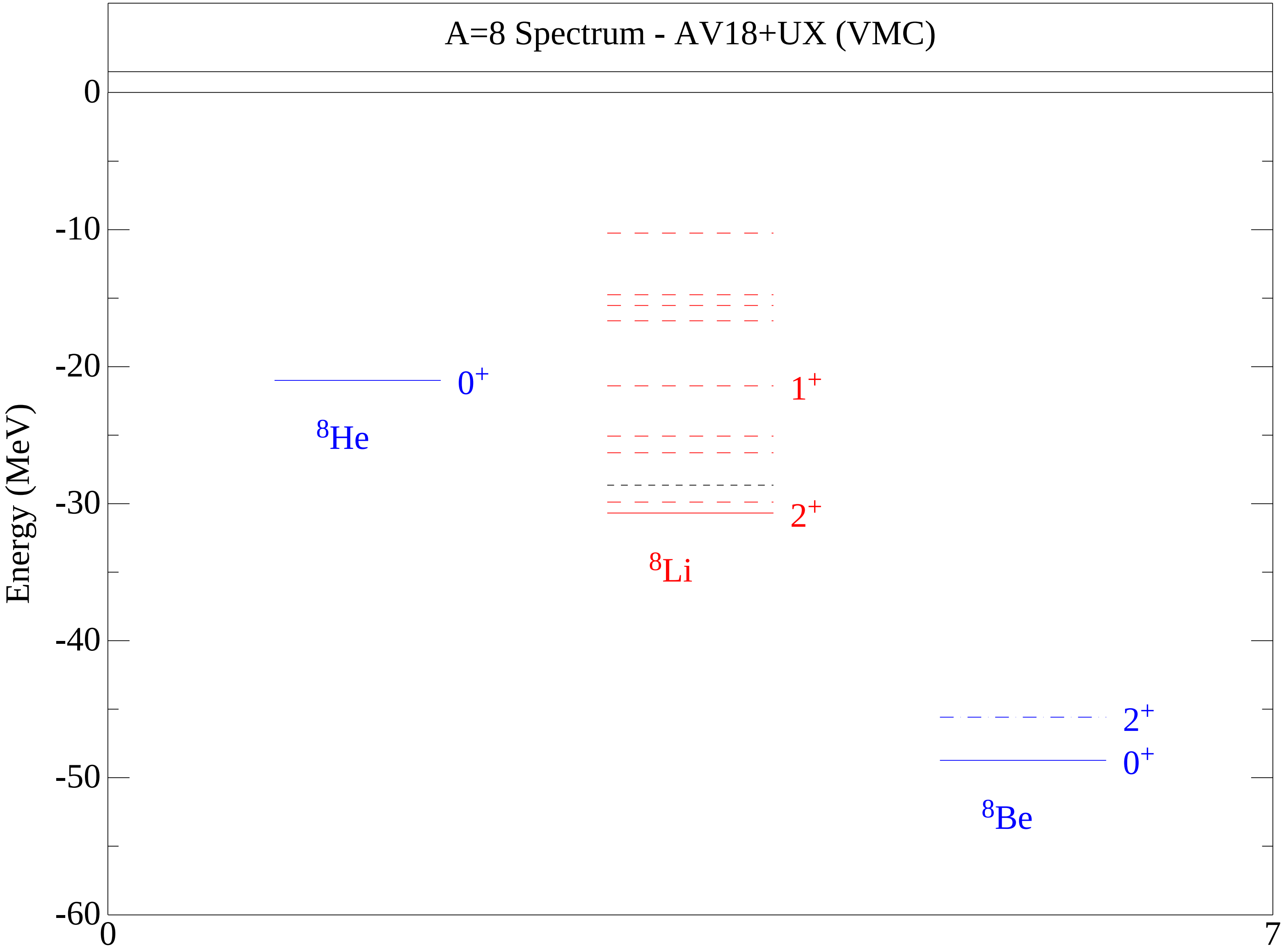
PRELIMINARY 0ν DOUBLE-BETA DECAY MATRIX ELEMENTS

$$O_V = \tau_1^+ \tau_2^+ / r_{12} \quad ; \quad O_A = \sigma_1 \cdot \sigma_2 \tau_1^+ \tau_2^+ / r_{12} \quad ; \quad O_T = S_{12} \tau_1^+ \tau_2^+ / r_{12}$$

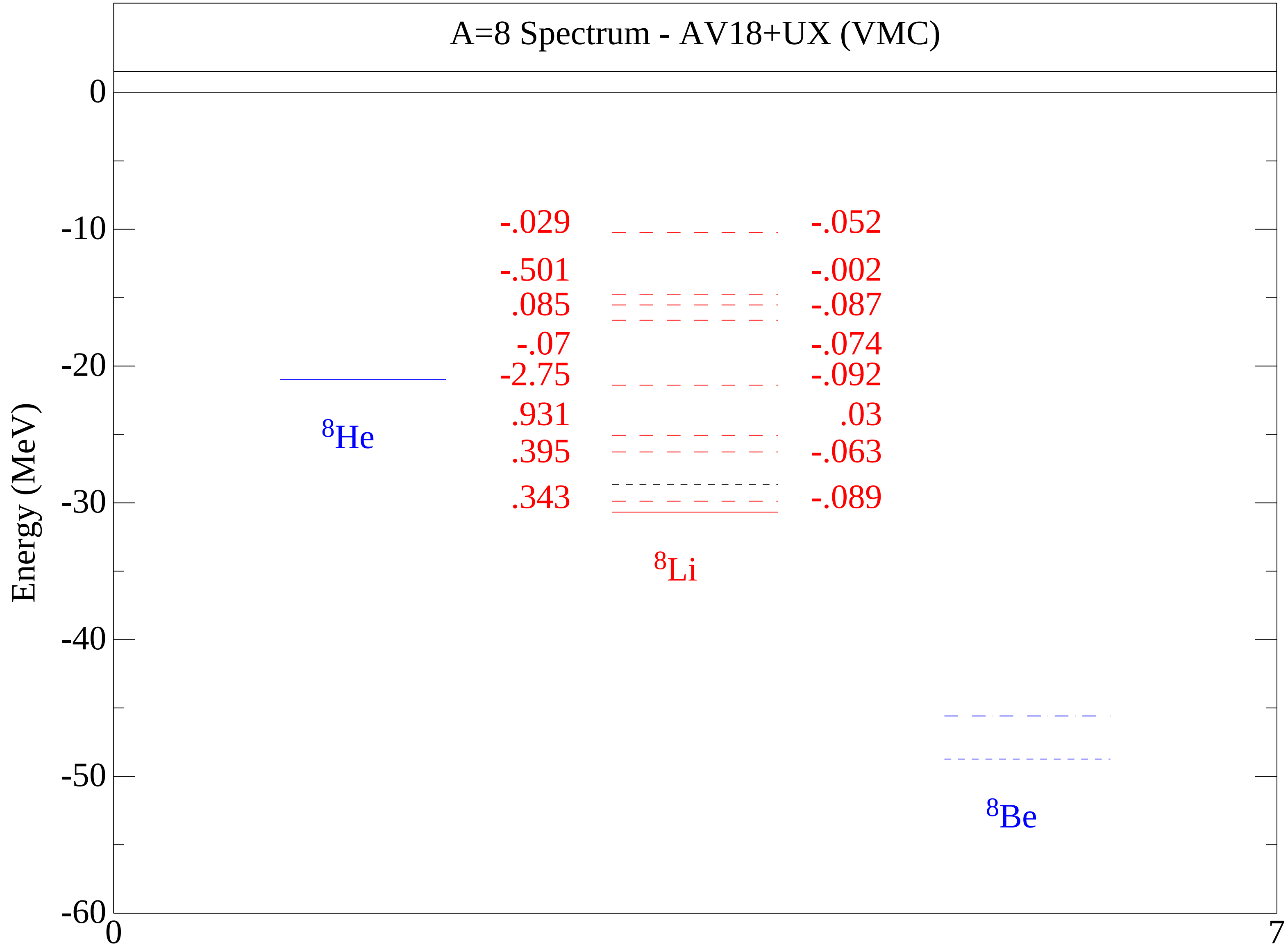
$\langle {}^8\mathrm{Be}(0^+;0) \vert O_x \vert {}^8\mathrm{He}(0^+;2) \rangle$	V	A	T
AV18+UX	0.0227(8)	-0.0368(14)	0.0298(10)
NV17-106	0.0288(4)	-0.0513(10)	0.0415(5)
$\langle {}^{10}\mathrm{Be}(0^+;1) \vert O_x \vert {}^{10}\mathrm{He}(0^+;3) \rangle$	V	A	T
AV18+UX	0.0174(7)	-0.0428(18)	0.0357(7)
NV17-106	0.0233(4)	-0.0575(10)	0.0645(8)
$\langle {}^{12}\mathrm{C}(0^+;0) \vert O_x \vert {}^{12}\mathrm{Be}(0^+;2) \rangle$	V	A	T
AV18+UX	0.055(2)	-0.137(4)	
NV17-106			


^{8}He(0^+;2) -> ^{8}Be(0^+;0) - AV18+UX
0.008
0.004
0.000
-0.004
-0.008
-0.012
-0.016
0
1
2
3
4
5
r (fm)
$\rho_{12}(r)$ (fm^{-3})
$\rho_V = \tau^+_1\tau^+_2 / r_{12}$
$\langle\psi_{Jf}|\rho_V|\psi_{Ji}\rangle$ = .0406
$\langle\psi_f|\rho_V|\psi_i\rangle$ = .0227
$\rho_T = S_{12}\,\tau^+_1\tau^+_2 / r_{12}$
$\langle\psi_f|\rho_T|\psi_i\rangle$ = .0298
$\langle\psi_{Jf}|\rho_T|\psi_{Ji}\rangle$ = 0
$\rho_A = \sigma_1\bullet\sigma_2\,\tau^+_1\tau^+_2 / r_{12}$
$\langle\psi_f|\rho_A|\psi_i\rangle$ = -.0368
$\langle\psi_{Jf}|\rho_A|\psi_{Ji}\rangle$ = -.122

WHAT ABOUT 2ν DOUBLE-BETA DECAY?



BASIS FOR 2ν DOUBLE-BETA DECAY CALCULATION?



CONCLUSIONS

- Accurate quantum Monte Carlo calculations up to $A \leq 12$ available for realistic nuclear Hamiltonians, including new local chiral Δ-ful models
- Energies and low-lying transitions in good agreement with experiment
- Variety of benchmark calculations for $\beta\beta$ decay are possible, including MEC (see Pastore talk)
- QMC calculations for larger nuclei to be made by AFDMC method, possibly starting with β decay in $A = 15, 17, 39, 41$ (see Carlson talk)

HAVE GUN WILL TRAVEL

WIRE PALADIN
SAN FRANCISCO

HAVE WAVE FUNCTIONS — WILL COLLABORATE