Nuclear and Nucleon Matter Constraints on Three-Nucleon Forces

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WORK NOT POSSIBLE WITHOUT EXTENSIVE COMPUTER RESOURCES

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Physics Division

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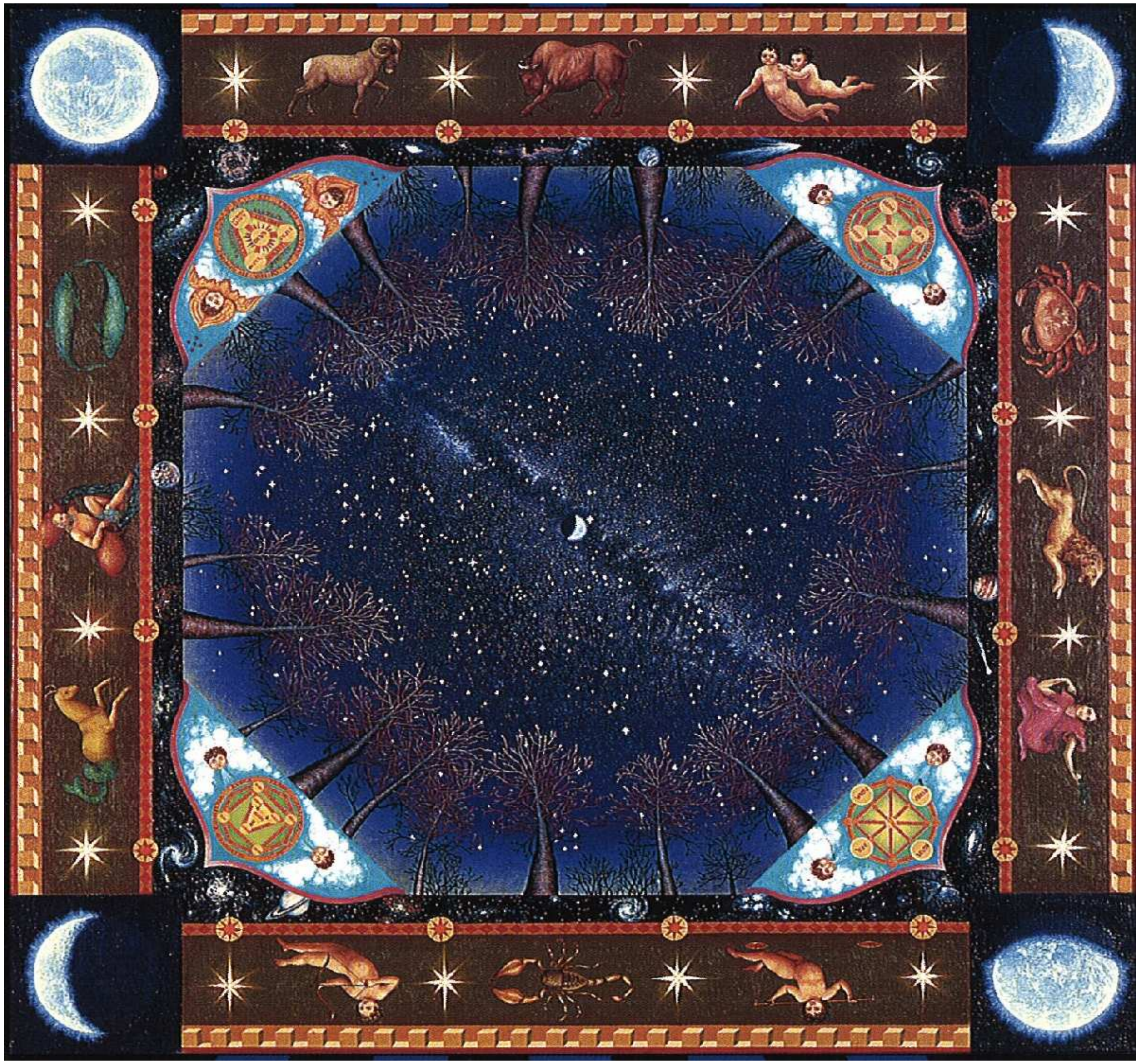


Night Sky Mandala

Oil on linen 36 x 36 inches

Leslie Morgan 1994

Ab Initio Calculations of Nuclei and Nucleon Matter

Goals

Understand nuclei & matter at level of elementary interactions between individual nucleons:

- Binding energies, excitation spectra, relative stability, matter saturation
- Densities, electroweak properties, transitions, neutron star mass & radii
- 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

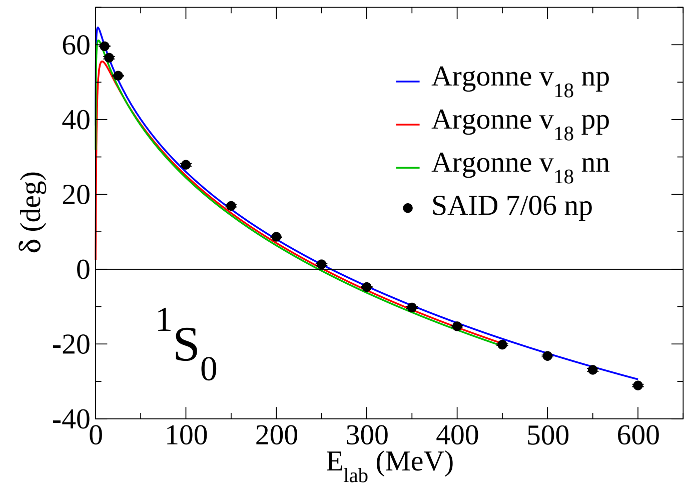
- Quantum Monte Carlo methods evaluate realistic Hamiltonians accurate to $\sim$1–2%
- About 100 states calculated for $A \leq 12$ nuclei in good agreement with experiment
- Electromagnetic moments, $M1$, $E2$, F, GT transitions, electroweak response
- Nucleon matter evaluated with Variational Chain Summation methods and/or AFDMC

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

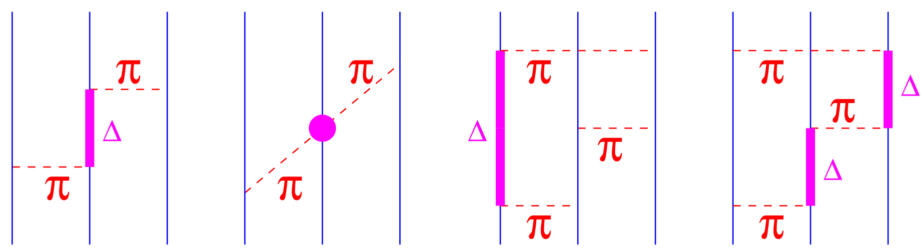
Argonne v$_{18}$: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij}) O_{ij}^p$



- 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**, 38 (1995)

Urbana & Illinois: $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{3\pi} + V_{ijk}^{R}$



- Urbana has standard 2π P-wave + one central short-short range repulsive term for nuclear 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 NV2: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{2\pi} + v_{ij}^{CT} = \sum v_p(r_{ij}) O_{ij}^{p}$

- derived in chiral effective field theory with Δ-intermediate states
- 16 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 different regularization fit to Granada PWA2013 data
- Ia,b fit to $\mathrm{E_{lab}}$ = 125 MeV with χ^2/d.o.f.$\sim$1.1
- IIa,b fit to $\mathrm{E_{lab}}$ = 200 MeV with χ^2/d.o.f.$\sim$1.4

Piarulli, Girlanda, Schiavilla, Kievsky, Lovato, Marcucci, Pieper, Viviani, & Wiringa PRC **94**, 054007 (2016)

Norfolk NV3: $V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^{CT}$

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

Piarulli, Baroni, Girlanda, Kievsky, Lovato, Marcucci, Pieper, Schiavilla, Viviani, & Wiringa PRL **120**, 052503 (2018)

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
- optimization code COBYLA used to search parameters

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; $\Psi(\tau) = \Psi_V + \delta\psi(\tau)$ and neglect $O(\delta\psi(\tau)^2)$

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

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

- Cannot propagate p^2, L^2, or $(\mathbf{L} \cdot \mathbf{S})^2$ operators $\Rightarrow$ 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

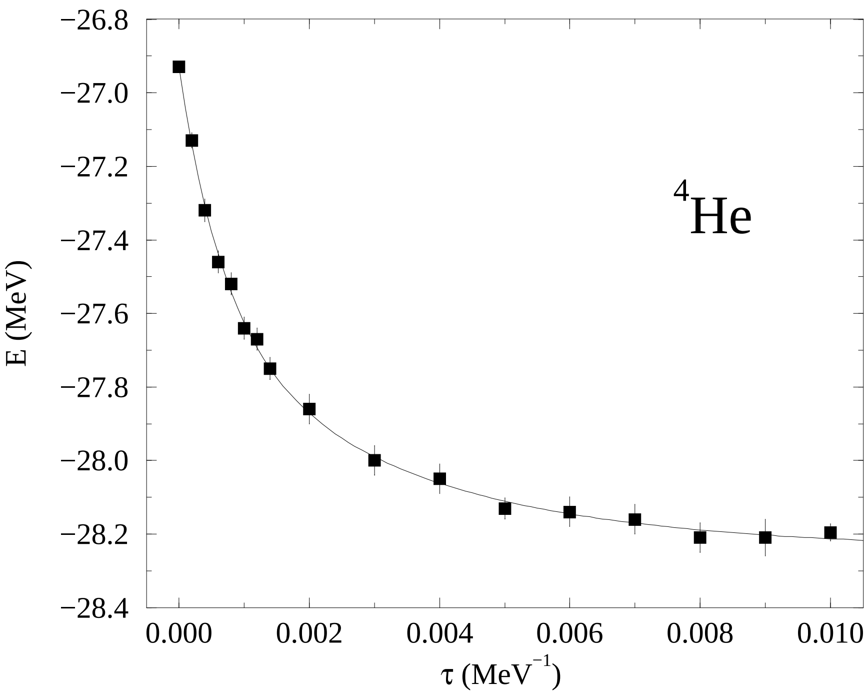
Carlson, PRC **38**, 1879 (1988)

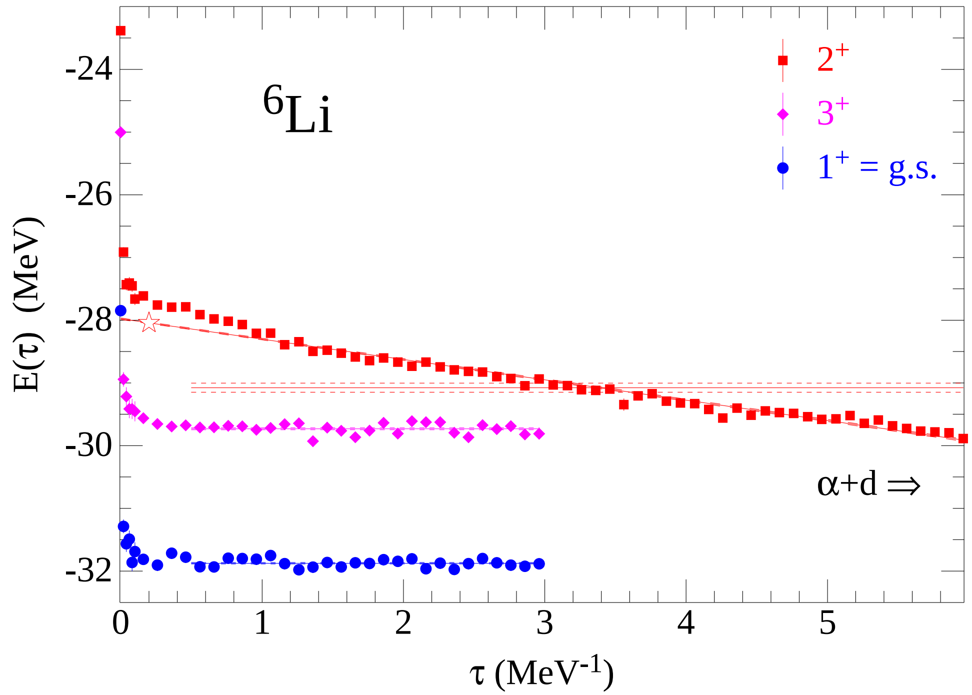
Pudliner, Pandharipande, Carlson, Pieper, & Wiringa, PRC **56**, 1720 (1997)

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

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

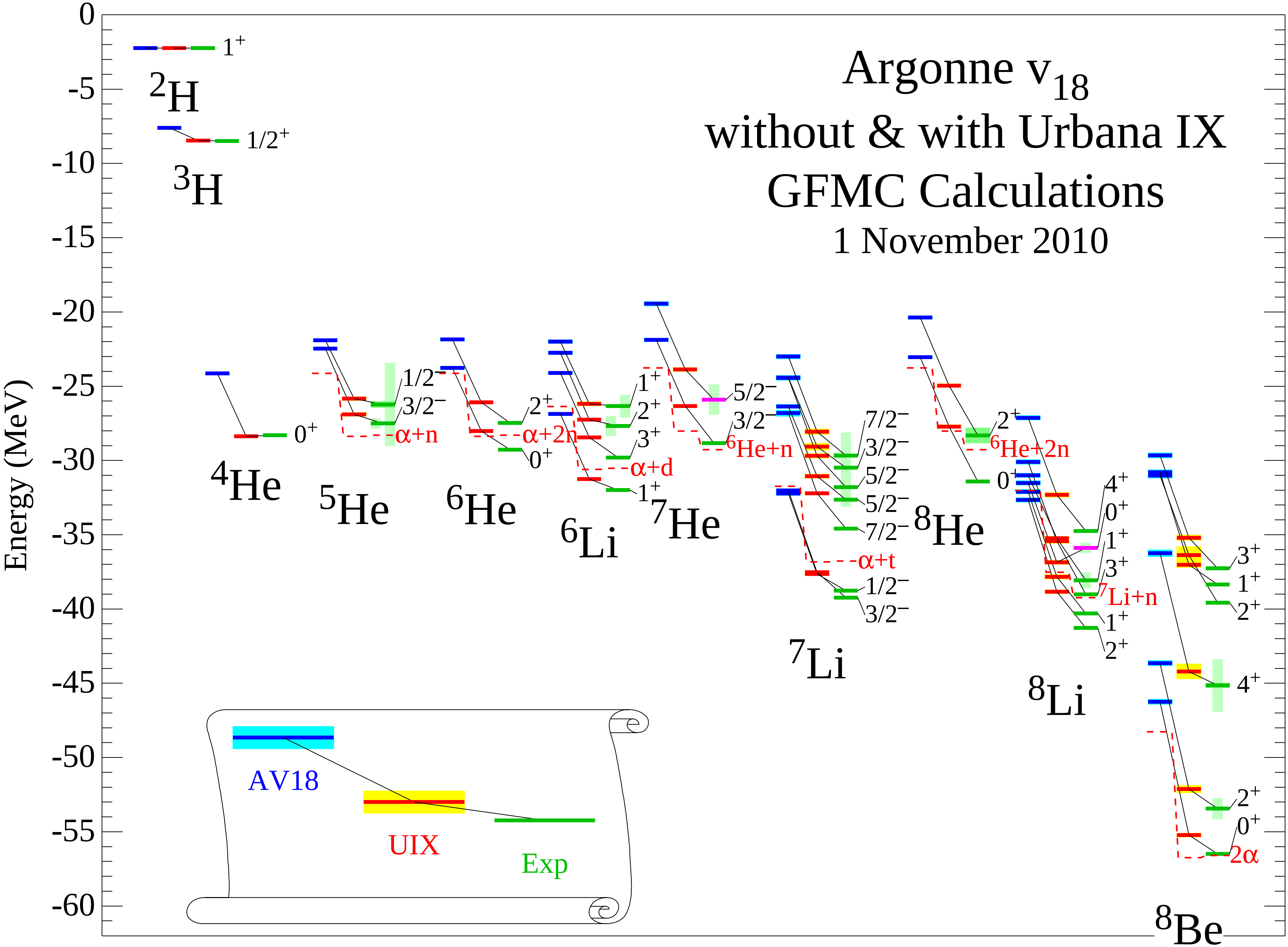
Examples of GFMC Propagation



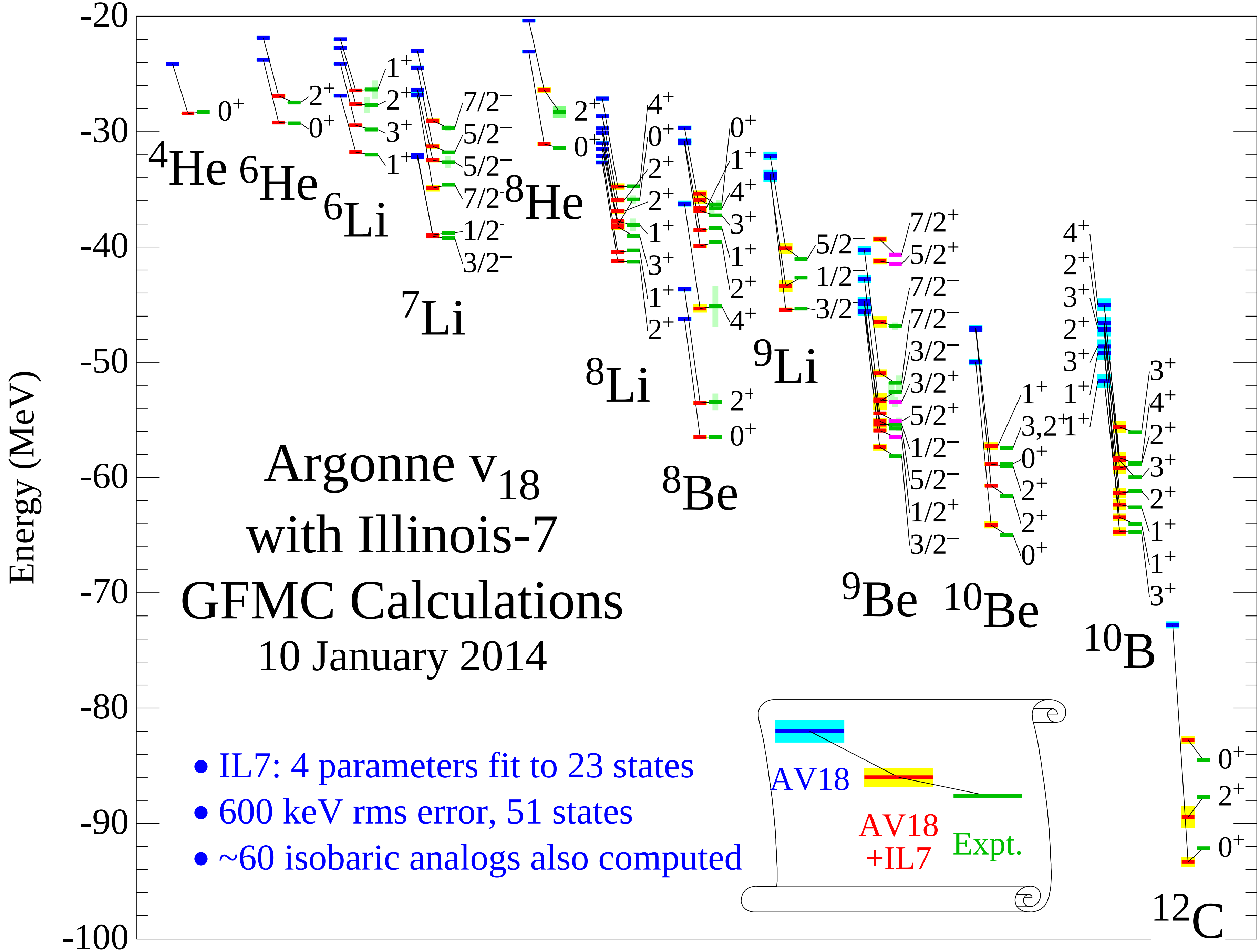


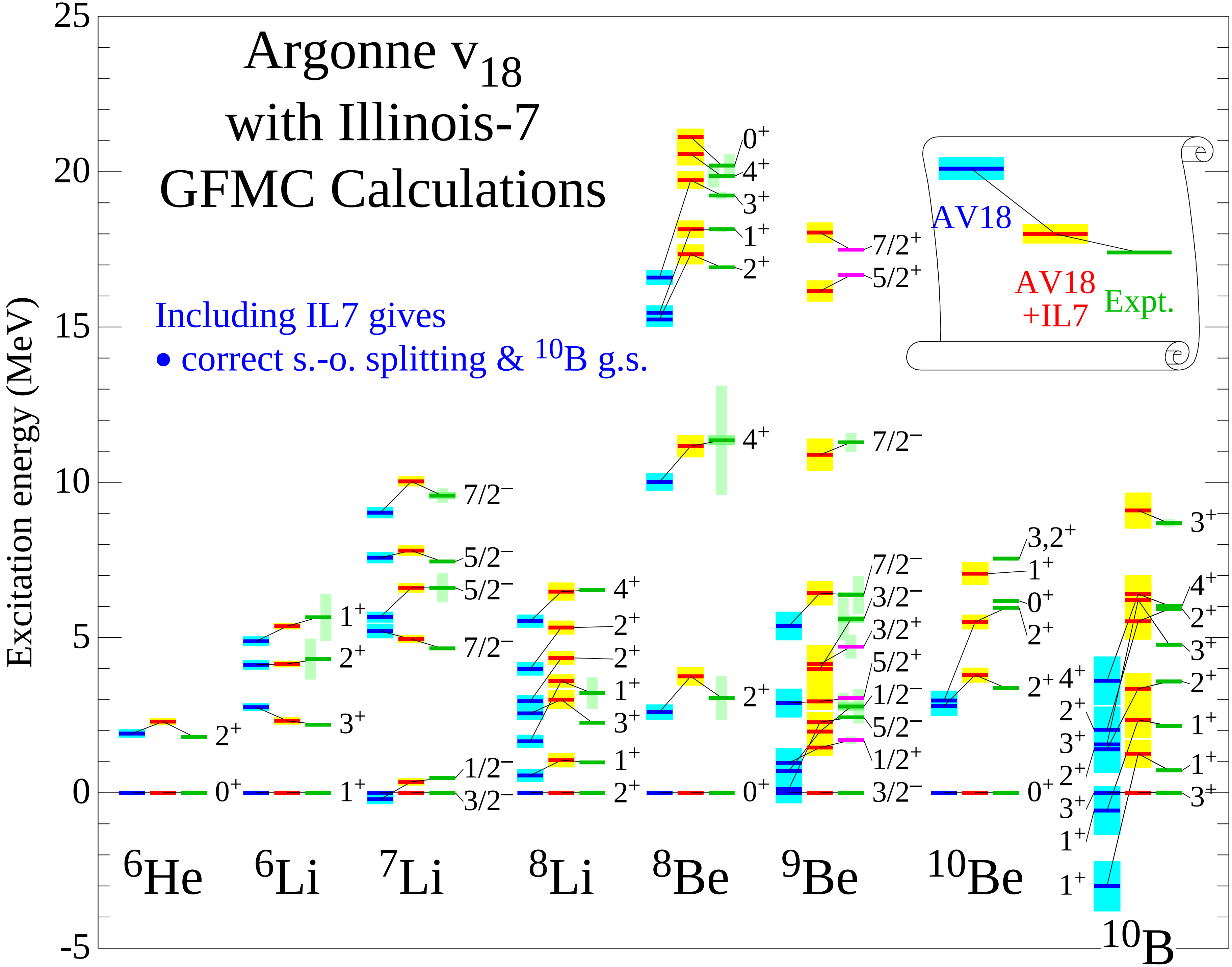
- Curve has $\sum_i a_i \exp(-E_i\tau)$ with E_i = 1480, 340 & 20.2 MeV (20.2 MeV is first ^{4}He 0^+ excitation)
- Ψ_V has small amounts of 1.5 GeV contamination

- 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

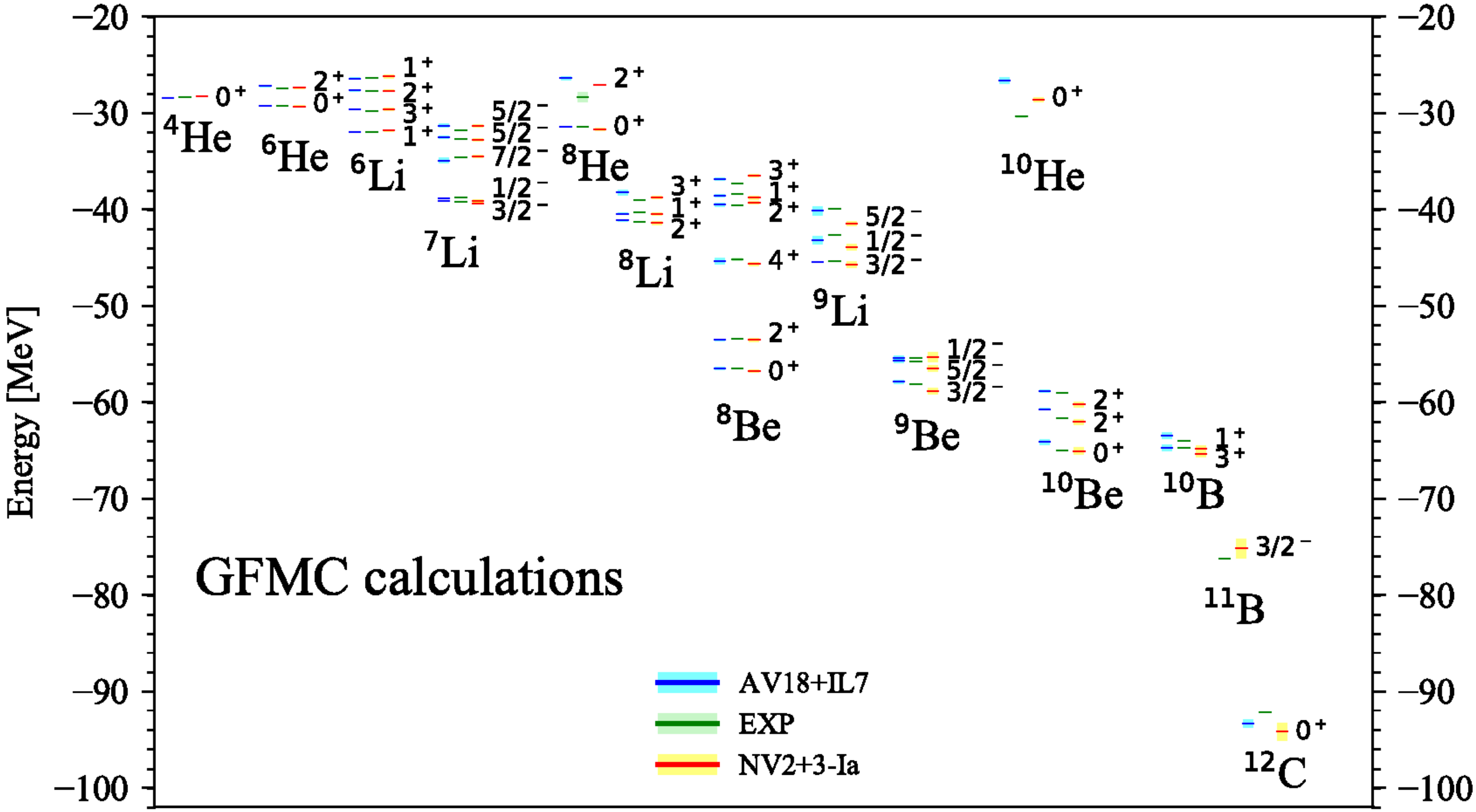


Argonne v18
without & with Urbana IX
GFMC Calculations
1 November 2010
Energy (MeV)
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
2H
3H
4He
5He
6He
6Li
7He
7Li
8He
8Li
8Be
α+n
α+2n
α+d
6He+n
α+t
6He+2n
7Li+n
2α
AV18
UIX
Exp


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
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.



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



RMS ΔE for 36 states: AV18+IL7 = 0.80 MeV ; NV2+3-Ia = 0.72 MeV
with signed average deviation: -0.23 MeV and +0.15 MeV

VMC Energy Expectation Values

^{4}He	$T_i + V_{ij}$	$V_{ijk}^{2\pi}$	V_{ijk}^{cD}	V_{ijk}^{cE}
NV2+3-Ia	−23.15	− 4.70	−3.77	4.28
NV2+3-Ib	−21.44	−10.10	2.64	1.90
NV2+3-IIa	−24.12	− 4.56	−1.29	2.89
NV2+3-IIb	−23.57	−10.49	6.06	0.90
AV18+UX	−22.56	− 8.79		3.79
AV18+UXI	−22.64	− 8.90	1.80	1.98

^{6}Li	$T_i + V_{ij}$	$V_{ijk}^{2\pi}$	V_{ijk}^{cD}	V_{ijk}^{cE}
NV2+3-Ia	−24.18	− 5.15	−4.50	4.48
NV2+3-Ib	−21.83	−10.66	2.99	2.06
NV2+3-IIa	−25.27	− 4.91	−1.58	3.21
NV2+3-IIb	−24.46	−11.12	6.72	0.90
AV18+UX	−23.80	− 9.11		4.29
AV18+UXI	−23.39	− 9.40	2.03	2.28

OBSERVATIONS FROM LIGHT NUCLEI RESULTS

- The $T_i + v_{ij}$ for all models underbind the light nuclei so need net attraction from V_{ijk}
- The $V^{2\pi}_{ijk}$ is attractive in all cases
- The net short-range V_{ijk} is usually repulsive
- The sign of NV3 c_D term is not well determined by binding energy alone
- The $\langle \tau_i \cdot \tau_k \rangle$ in NV3 c_E term is negative in light nuclei; will change sign in neutron matter
- The corresponding central term in Urbana models is repulsive in light nuclei & matter
- This short-short range term in Urbana V_{ijk} gets most of its contribution by connecting $S = \frac{1}{2}$ to $S = \frac{1}{2}$ and $S = \frac{3}{2}$ to $S = \frac{3}{2}$ triples
- The π-short range term in UXI gets most of its contribution by connecting $S = \frac{1}{2}$ to $S = \frac{3}{2}$ triples so is sensitive to tensor correlations

VARIATIONAL CHAIN SUMMATION

Variational energy expectation value of infinite many-body system can be written as:

$$E_V = \frac{\int \mathcal{A}(\prod_i \Phi_i^*) \, \mathcal{S}(\prod_{i<j} F_{ij}^\dagger) \; H \; \mathcal{S}(\prod_{i<j} F_{ij}) \, (\prod_i \Phi_i) \, d\tau}{\int \mathcal{A}(\prod_i \Phi_i^*) \, \mathcal{S}(\prod_{i<j} F_{ij}^\dagger) \; \mathcal{S}(\prod_{i<j} F_{ij}) \, (\prod_i \Phi_i) \, d\tau}$$

where $F_{ij} = \sum_p f^p_{ij} O^p_{ij}$ are correlation operators and $\Phi_i = \exp[i\mathbf{k_i} \cdot \mathbf{r_i}]$ are plane-wave states and for convenience only the l.h.s. Ψ^* is antisymmetrized.

This integral can be approximated by expading the dynamical correlations in powers of short-ranged functions $F^c_{ij} = F^1_{ij} = (f^c_{ij})^2 - 1$ and $F^{p>1}_{ij} = 2 f^c_{ij} f^{p>1}_{ij}$ and $f^{p>1}_{ij} f^{q>1}_{ij}$, and in powers of the statistical correlation (Slater function) $\ell(k_F r) = 3 j_1(k_F r)/(k_F r)$.

This expansion is conveniently represented by generalized Mayer diagrams and a very general diagrammatic expansion valid for noncommuting operators has been developed, commonly referred to as the Fermi hypernetted chain + single-operator chain (FHNC+SOC) method. Present calculations of central correlations are now beyond the "FHNC/4" level.

Pandharipande & Wiringa, RMP **51**, 821 (1979)
Wiringa, Fiks & Fabrocini, PRC **38**, 1010 (1988)

Akmal, Pandharipande & Ravenhall, PRC **58**, 1804 (1998)

Energy in FHNC calculations

The energy can be computed using distribution functions g and g_3 (in Pandharipande-Bethe form):

$$\begin{aligned} E_{PB} &= T_F + W + W_F + U + U_F \\ W &= \frac{\rho}{2}\int \left(v_{ij} - \frac{\hbar^2}{m}\frac{\nabla^2 f_{ij}}{f_{ij}} \right) g_{ij} d^3 r_{ij} \\ U &= -\frac{\hbar^2}{2m}\frac{\rho^2}{4}\int \left(\frac{\nabla_i f_{ij}\cdot\nabla_i f_{ik}}{f_{ij} f_{ik}} \right) g_3(\mathbf{r}_{ij},\mathbf{r}_{ik}) d^3 r_{ij} d^3 r_{ik} \end{aligned}$$

The two-body distribution function can be written as:

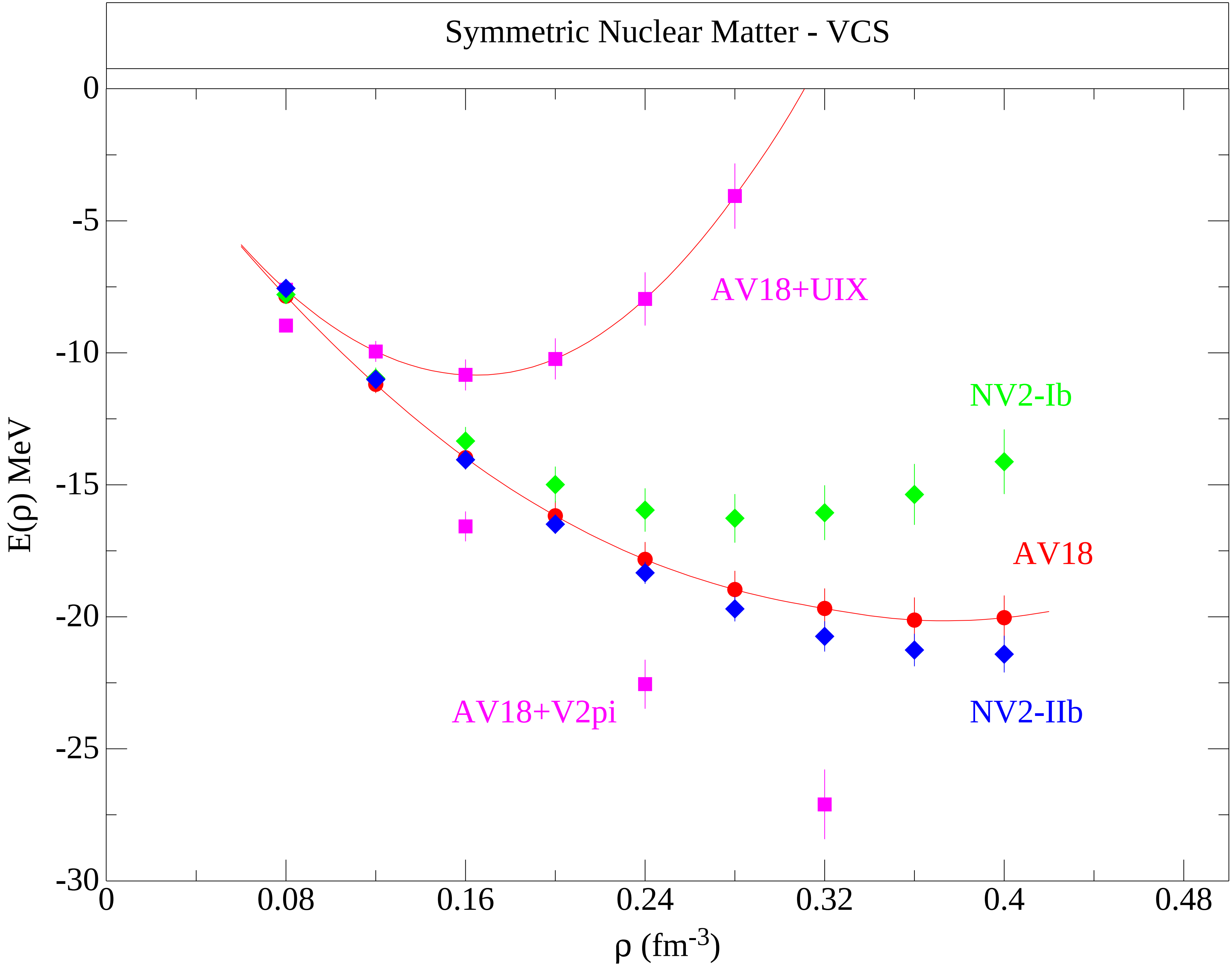
$$g_{ij} = f^2 \left[(1 + G_{de} + \mathcal{E}_{de})^2 + G_{ee} + \mathcal{E}_{ee} - \nu (G_{cc} + \mathcal{E}_{cc} - \ell/\nu)^2 \right] exp(G_{dd} + \mathcal{E}_{dd}) \; .$$

where the chain functions G_{xy} are sums of nodal diagrams, with direct (d), exchange (e) or circular exchange (c) end points and $\mathcal{E}_{xy}$ are elementary diagrams. A more complicated expression is available for g_3:

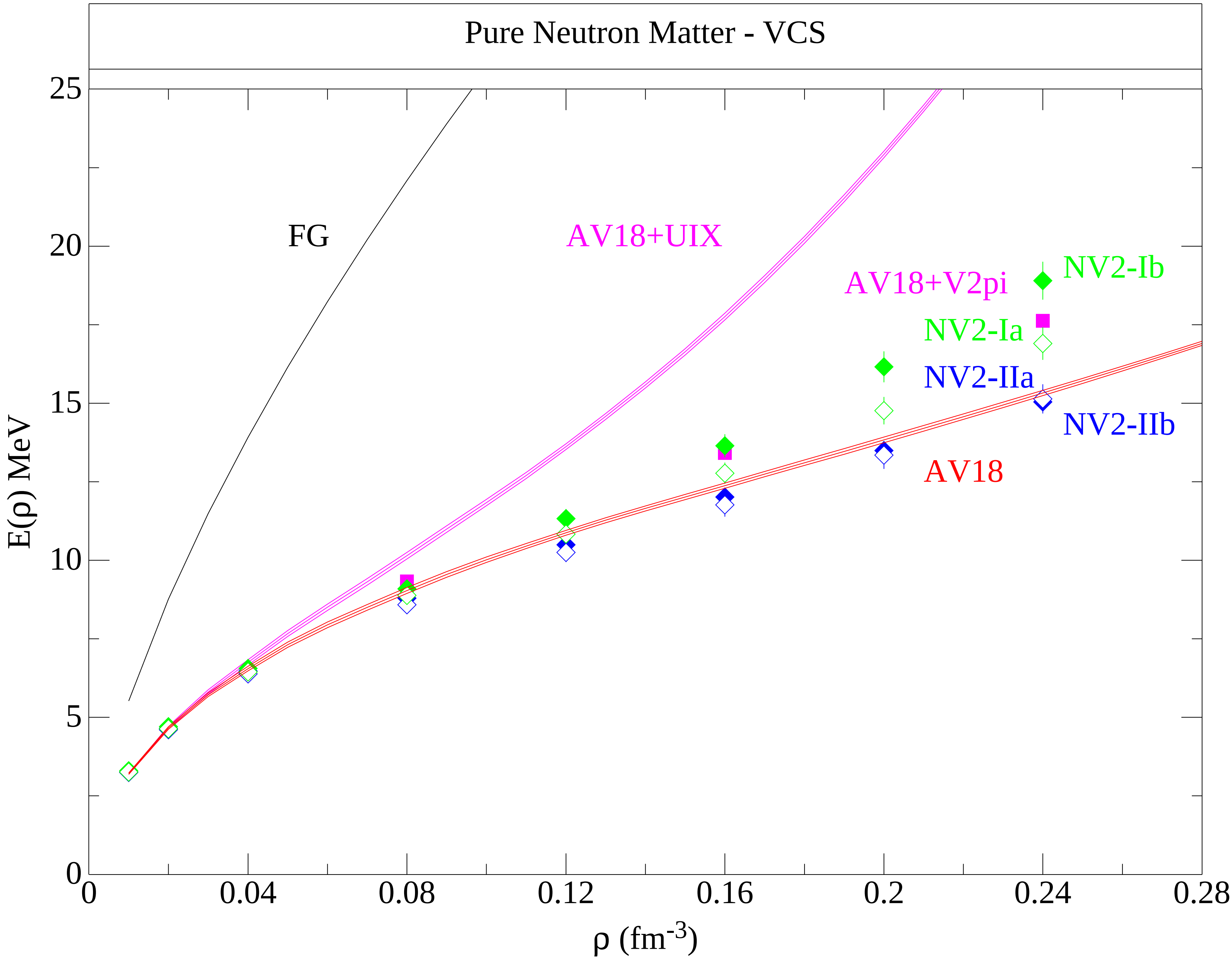
$$g_3(r_{ij}, r_{ik}, r_{jk}) = \sum_n A^n_{ij} B^n_{ik} C^n_{jk} D^n_{ijk}$$

Alternatively one can perform an integration by parts to get the Jackson-Feenberg form:

$$E_{JF} = \frac{\rho}{2}\int \left[v_{ij} - \frac{\hbar^2}{2m}\left(\frac{\nabla^2 f_{ij}}{f_{ij}} - \frac{(\nabla_i f_{ij})^2}{f^2_{ij}} \right) \right] g_{ij} d^3 r_{ij}$$



Symmetric Nuclear Matter - VCS
0
-5
-10
-15
-20
-25
-30
0
0.08
0.16
0.24
0.32
0.4
0.48
E(ρ) MeV
ρ (fm-3)
AV18+UIX
NV2-Ib
AV18
AV18+V2pi
NV2-IIb



Pure Neutron Matter - VCS
E(ρ) MeV
ρ (fm^{-3})
FG
AV18+UIX
AV18+V2pi
NV2-Ib
NV2-Ia
NV2-IIa
NV2-IIb
AV18
0
5
10
15
20
25
0
0.04
0.08
0.12
0.16
0.2
0.24
0.28

Observations from nuclear and neutron matter results

- Local two-nucleon interactions fit to NN data saturate symmetric nuclear matter (SNM) at $\approx 2\rho_0$
- $V_{ijk}^{2\pi}$ by itself is attractive in SNM and pushes saturation to even higher density
- Shorter-range V_{ijk} must provide net repulsion to saturate at empirical density
- For UIX this is all c_E-like; for UXI it is split between c_E- and c_D-like terms in same ratio as in light nuclei
- The NV2-II models fit to higher energy are closer to AV18 in both SNM and pure neutron matter (PNM)
- In PNM the $V_{ijk}^{2\pi}$ is weakly repulsive
- For UIX the dominant repulsion in PNM is central c_E-like term
- For UXI the c_D-like term is much reduced relative to c_E-like because of weak tesnor correlations
- A c_E term with $\tau_i \cdot \tau_k$ dependence is likely to be problemattic

Summary and Future Work

- NV2+3-Ia reproduces nuclear binding and excitation energies for $A \leq 12$ extremely well, comparable to AV18+IL7
- However, neither model looks able to support massive neutron stars
- Energy spectra for other NV2+3 models are being evaluated, but initial c_D and c_E choices do not give as promising results
- Determining c_D and c_E from ^{3}H binding and nd scattering fits is not easy because these data are highly correlated
- Alternate strategy is to include ^{3}H β decay information and energies of larger nuclei like ^{8}He, ^{8}Be, ^{10}B(3^+,1^+) states; another possibility is $n\alpha$ scattering data
- Many other electroweak transitions are being evaluated and may help select "best" models
- Nuclear and neutron matter provide additional constraints, even if the calculational methods are less precise than for light nuclei
- Meeting all these demands may well require including sub-leading terms in V_{1jk} with more spin-isospin operator dependence