QMC Calculations of Nuclei and Neutron Drops

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Work with

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- Hamiltonian and QMC methods
- GFMC ^{12}C progress
- VMC & GFMC scattering
- GFMC & AFDMC for neutron drops
- GFMC for nuclear overlaps (Brida)
- GFMC breakdown of V_{ijk}
- Deliverables and plans

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Physics Division

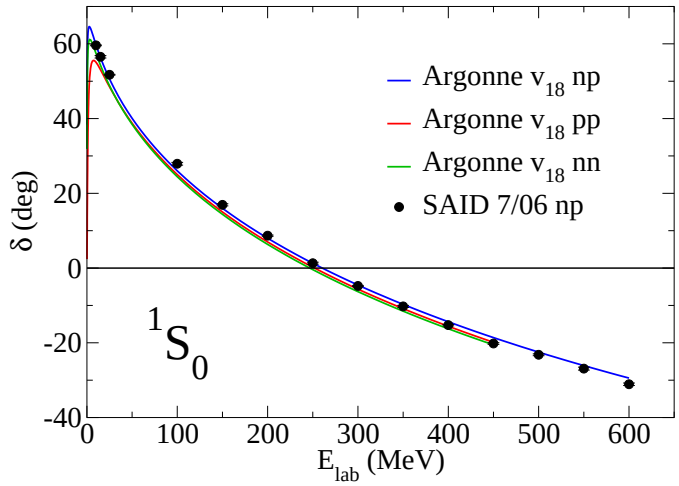
NUCLEAR HAMILTONIAN

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

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

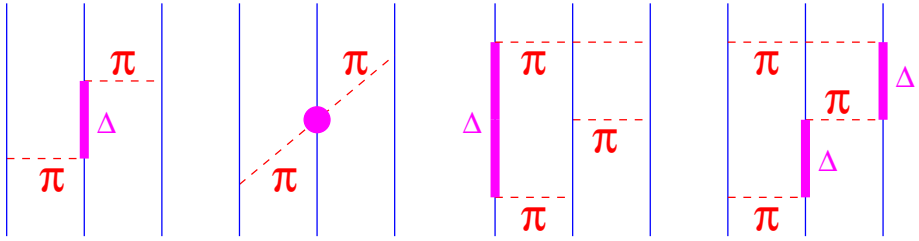
Argonne v$_{18}$: $v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{I} + v_{ij}^{S} = \sum v_p(r_{ij}) O_{ij}^{p}$

- predominantly local operator structure – good for QMC
- EM and strong CD and CSB terms included
- fits Nijmegen PWA93 data base with χ^2/d.o.f.=1.1
- qualitatively good to ~1 GeV



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)

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 $E_V = \langle \Psi_V | H | \Psi_V \rangle \geq E$

These are $\sim 2^A \binom{A}{Z}$ component (270,336 for ^{12}C) spin-isospin vectors in $3A$ dimensions

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 $A \geq 5$
- Multiple excited states for same J^π stay orthogonal

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

Wiringa, Pieper, Carlson, & Pandharipande, PRC **62**, 014001 (2000)
Pieper, Varga, & Wiringa, PRC **66**, 044310 (2002)
Pieper, Wiringa, & Carlson, PRC **70**, 054325 (2004)
Pieper, NPA **751**, 516c (2005)

Quantum Monte Carlo (continued)

Auxiliary field diffusion Monte Carlo (AFDMC):

- Use Hubbard-Stratonovich transformation to linearize propagator spin-isospin dependence

$$e^{\frac{1}{2}\Delta\tau O^2} = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-\frac{x^2}{2} + x\sqrt{\Delta\tau}O}$$

- Sample spin states with auxiliary fields x instead of complete summation
- Starting Ψ_V must be simpler - no spin or tensor correlations
- Operators other than energy harder to compute
- Computation does NOT grow exponentially with size of system

Systems of up to 114 neutrons in a box have been evaluated.

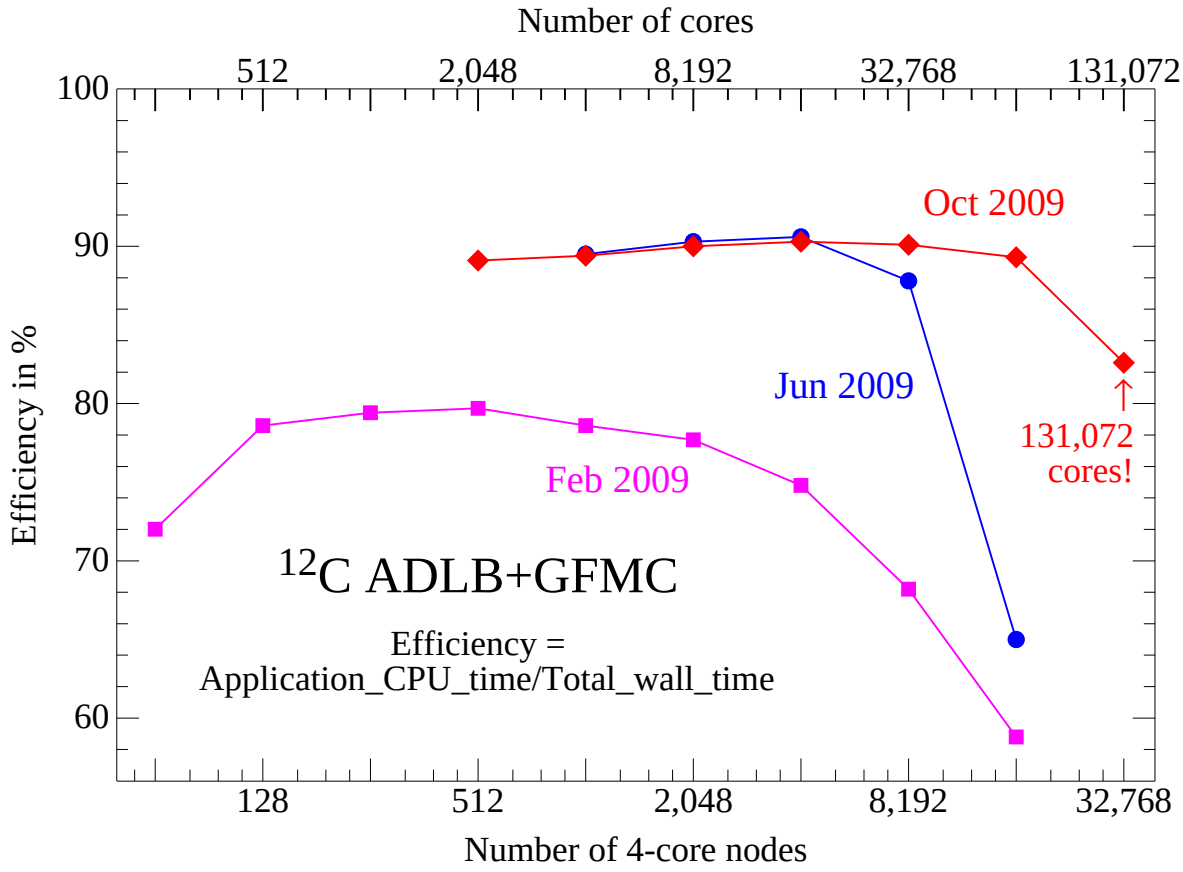
Sarsa, Fantoni, Schmidt, & Pederiva, PRC **68**, 024308 (2003)
Gandolfi, Pederiva, Fantoni, & Schmidt, PRL **98**, 102503 (2007)
Gandolfi, Illarionov, Schmidt, Pederiva, & Fantoni, PRC **79**, 054005 (2009)

MAKING GFMC WORK ON 131,072 PROCESSORS AND ^{12}C

Work with Mathematics & Computer Science Division under UNEDF SciDAC

- General purpose load balancing library (ADLB) developed to run under MPI
  - GFMC code is driver and testbed
  - Achieves 82% efficiency on 32,768 nodes of Argonne's IBM Blue Gene/P
- Open MP used for 4 cores on each node = 131,072 processors total

ADLB performance is very good up to 32,768 nodes (131,072 cores)



An Alternative Implementation of ADLB

No change to the API.

Utilize the memory and computing resources of all clients.

Use a single server to manage global state, thus freeing up servers to become clients and do useful work. Eliminates race conditions on global state.

Use MPI one-sided operations (Put/Get) to allow clients to put/get work units into/from other clients while they are working.

Status:

- Found bugs in one-sided MPI implementation on both BG/P and Infiniband Cluster; fixed.
- Single server algorithm seems to be impacting scalability more than expected.
- Experiments are ongoing.

^{12}C(0^+) Trial Wave Functions

The Jastrow part of Ψ_V for J=0^+ states is a major part of the entire calculation.

There are 5 LS-basis J=0^+ states in ^{12}C in the $0P$ shell:
^{1}S[444], ^{3}P[4431], ^{1}S[4422], ^{5}D[4422], ^{3}P[4332]

Only the ^{1}S[444] can be directly constructed in reasonable computer time. Carlson found a way to construct all 5 states by projection from a closed $(p3/2)^8$ state.

^{12}C states have strong triple-alpha structure; Pandharipande made a subroutine that explicitly makes triple-alpha states with one α in the $0S$ shell and two in the $0P$ shell.

Last year we reported results for the ground state using both the AV18 and AV18+IL7 Hamiltonians – the latter in excellent agreement with experiment for energy and density.

SECOND 0^+ (HOYLE) STATE OF ^{12}C – SO FAR

The second 0^+ state of ^{12}C is the famous triple-alpha burning or Hoyle state

- Resonance only 0.38 MeV above 3α breakup threshold
- Doorway state postulated by Fred Hoyle for $3\alpha \rightarrow {}^{12}$C in stars
- Shell model calculations show it to be 4-particle 4-hole excitation
- Not yet converged in *ab initio* no-core shell model.
- We add Pandharipande triple-α component to Ψ_V with α's in $0S$ shell, $0P$ shell, and $1S$-$0D$ shell
- We also try only a pair in $1S$-$0D$ shell, i.e., an α made of $0P^2 0D^2$ or $0P^2 1S^2$
- The $1S$-$0D$ shell one-body $\phi(r)$ are given a large RMS radius

One example of the diagonalization

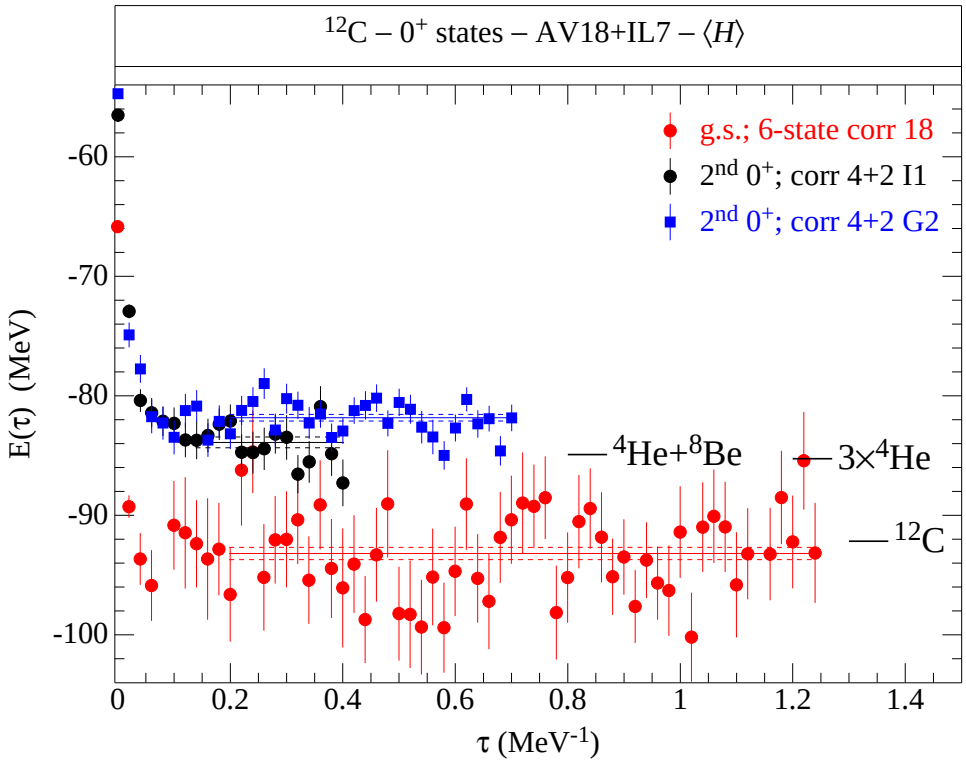
	3-α states*				LS $0P$ shell states				
	$0P^4$	$0D^4$	$1S^4$	$0D^2 1S^2$	^{1}S[444]	^{3}P[4431]	^{1}S[4422]	^{5}D[4422]	^{3}P[4332]
gs	43.%	0.0%	0.0%	0.6%	42.%	14.%	0.015%	0.39%	0.10%
$2^{\rm nd}$ 0^+	12.%	62. %	1.0%	5.6%	18.%	1.5%	0.13%	0.0%	0.05%

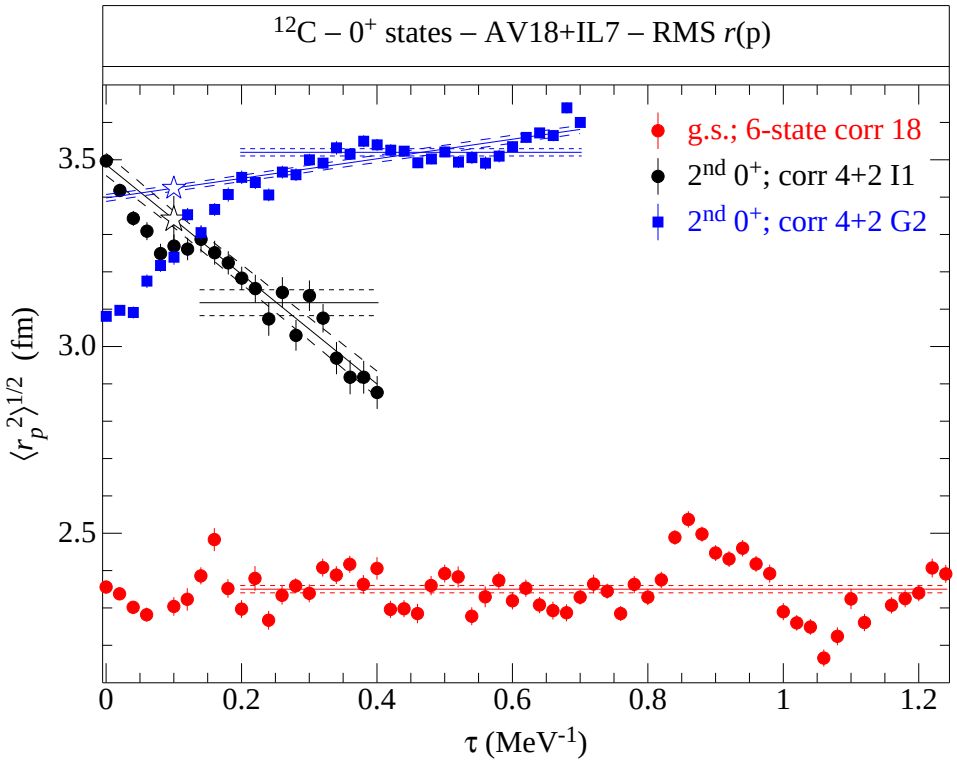
* Shells of the last α are shown

Because of the very different RMS radii, accurate diagonalizations are difficult

Second 0^+ (Hoyle) State of ^{12}C – so far

Convergence as a function of imaginary time (τ)



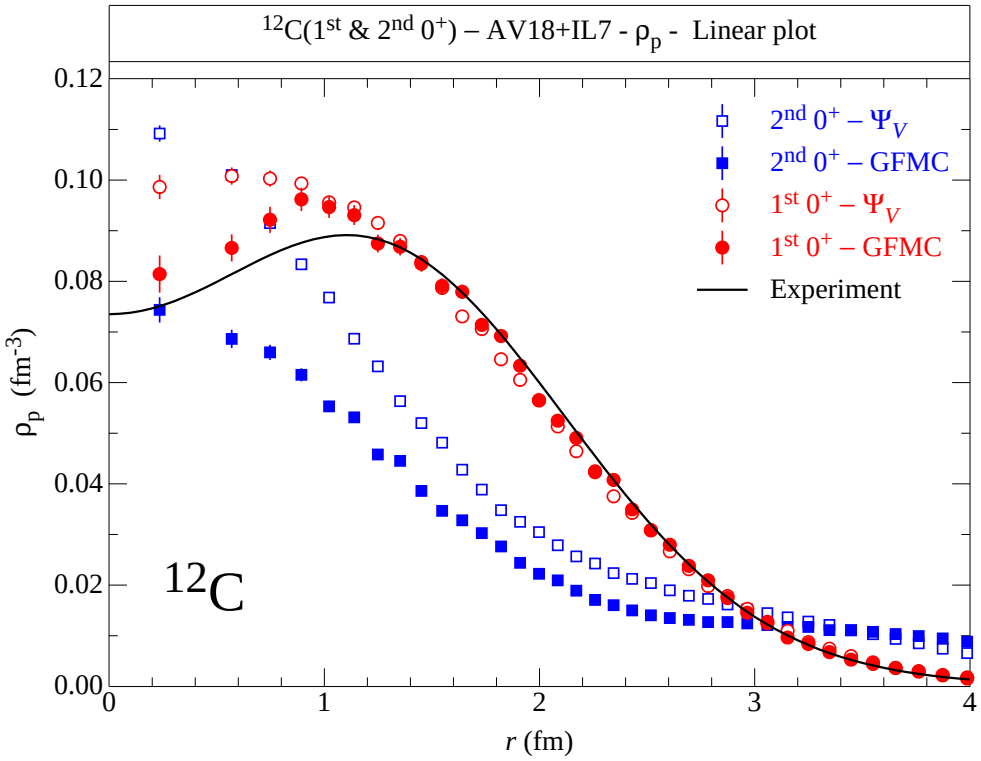


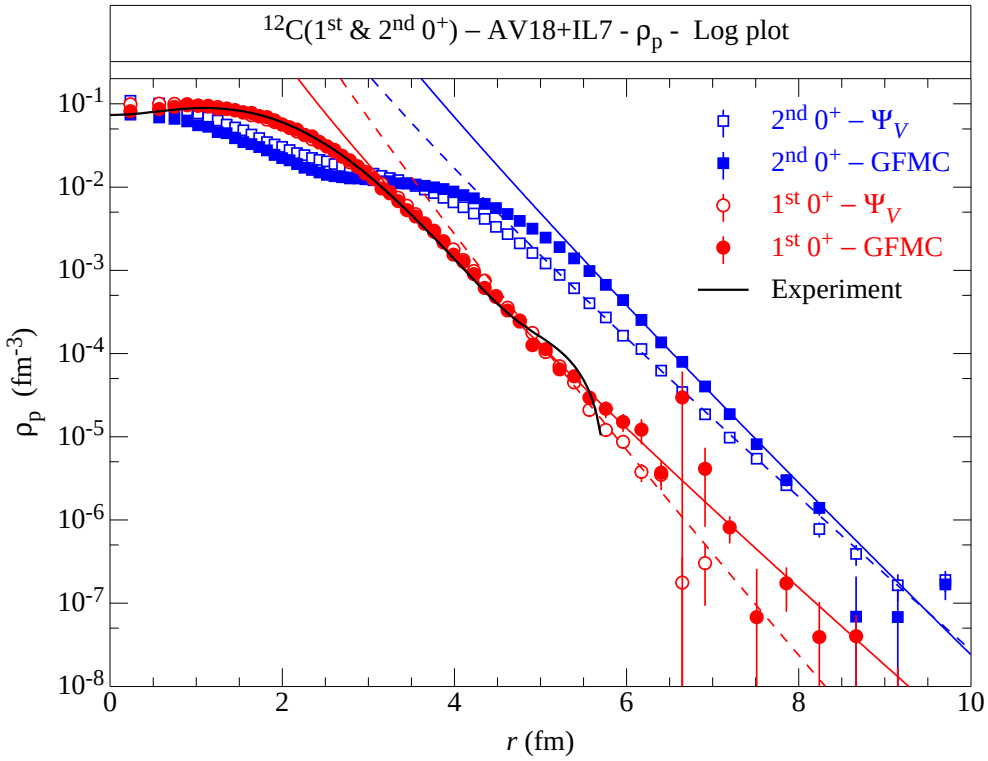
Statistical errors are too large to rediagonalize GFMC at each time step

	g.s. energy		2^{nd} 0^+ E^*	
	GFMC	Expt.	GFMC	Expt.
AV18	–72.8(3)		7.5(5)	
AV18+IL7	–93.2(6)	–92.16	11.3(7)	7.65

SECOND 0^+ (HOYLE) STATE OF ^{12}C – SO FAR

One-body density





- Ground-state $\rho(r)$ has dip at $r = 0$ – suggests(?) equilateral triangle of 3 α's
- $2^{\rm nd}$ 0^+ $\rho(r)$ has no dip at $r = 0$ – suggests(?) $\sim$ line of 3 α's

GFMC FOR SCATTERING STATES

GFMC calculations for particle-stable systems have exponentially decaying asymptotic boundary conditions – adequate also for energies of narrow resonances

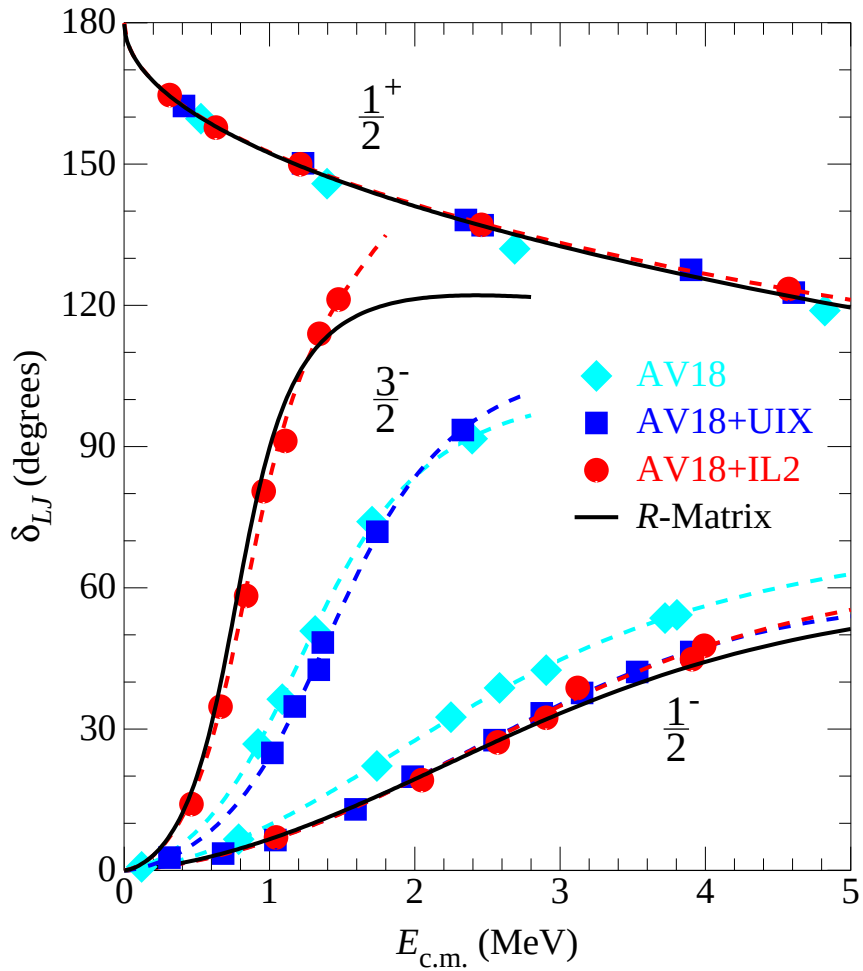
For locations and widths of wide states need to do true scattering:

- 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_B, finds $E(R_B, \chi)$
- Phase shift, $\delta(E)$, is function of R_B, χ, E
- Repeat for multiple χ to map out $\delta(E)$
- need E accurate to $\sim 1/3\%$

^{5}He as n–^{4}He scattering

Black curves: Hale phase shifts from R-matrix data analysis up to $J = \frac{9}{2}$

AV18+IL2 reproduces the S-wave scattering length and locations and widths of both P-wave resonances

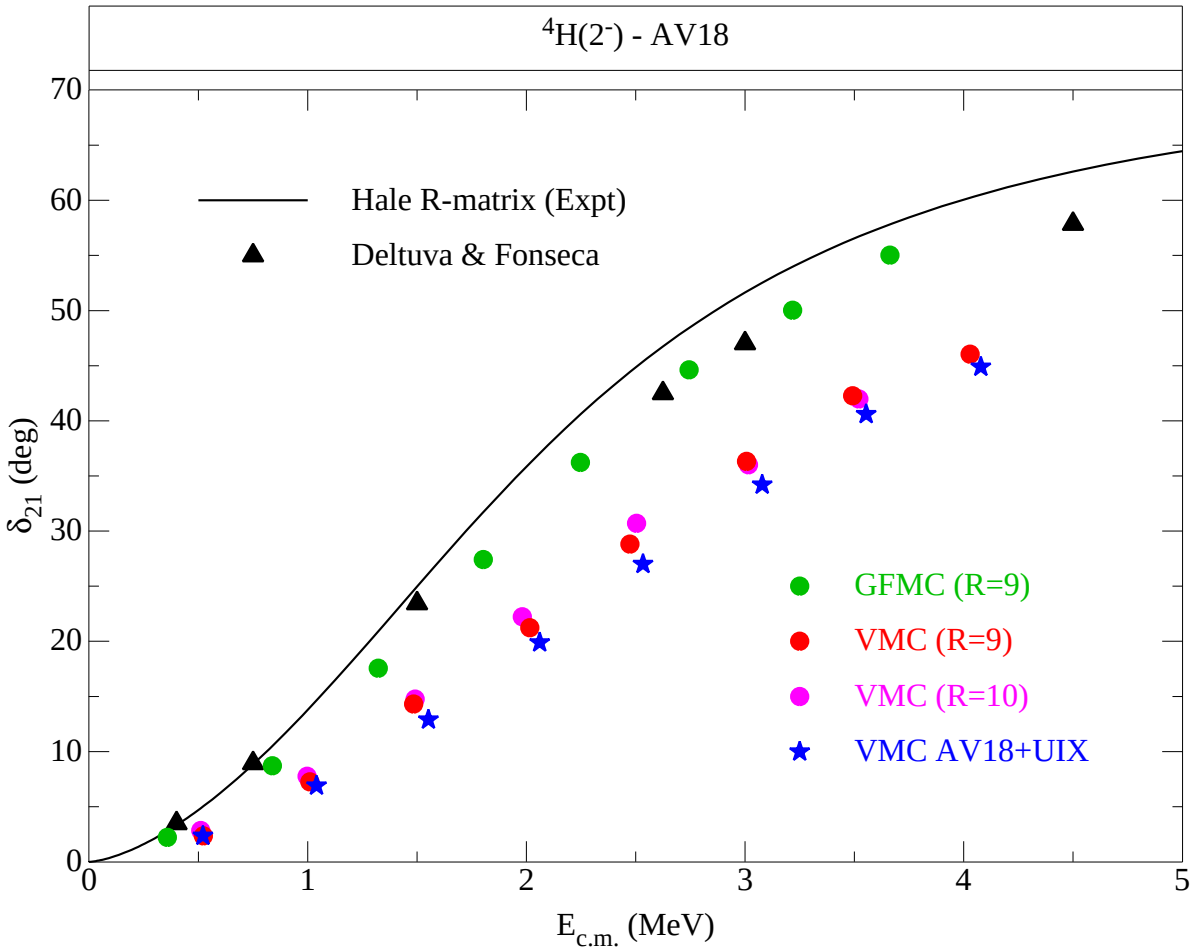


Nollett, Pieper, Wiringa, Carlson, & Hale,
PRL **99**, 022502 (2007)

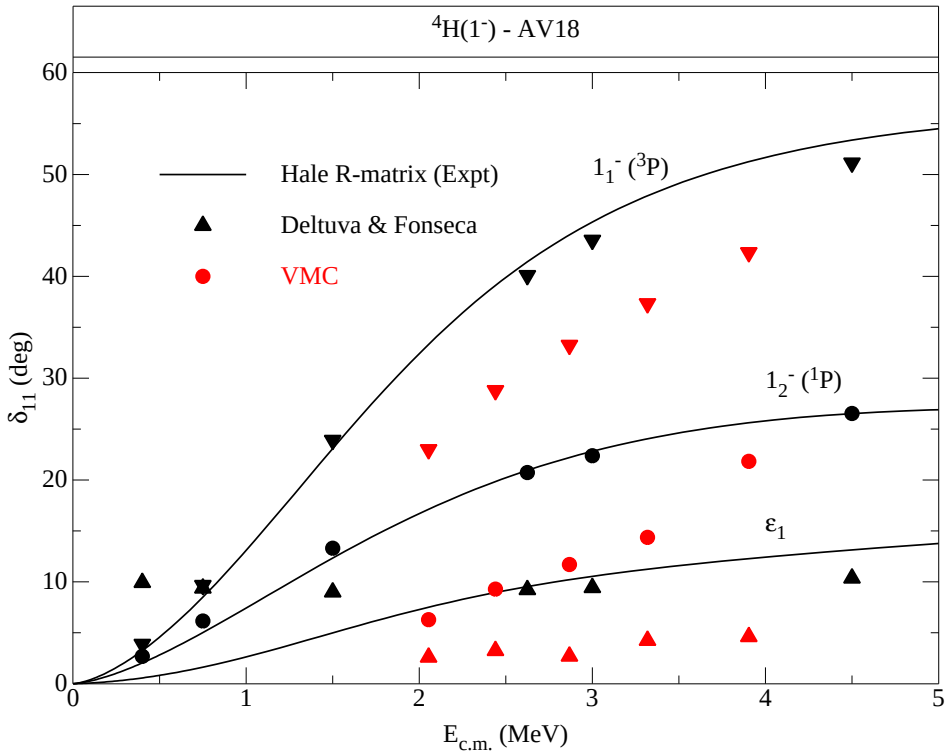
Application for NIST spin-rotation experiment:
$\langle \Psi_{n\alpha}(1/2^-)|H_{PV}|\Psi_{n\alpha}(1/2^+)\rangle$

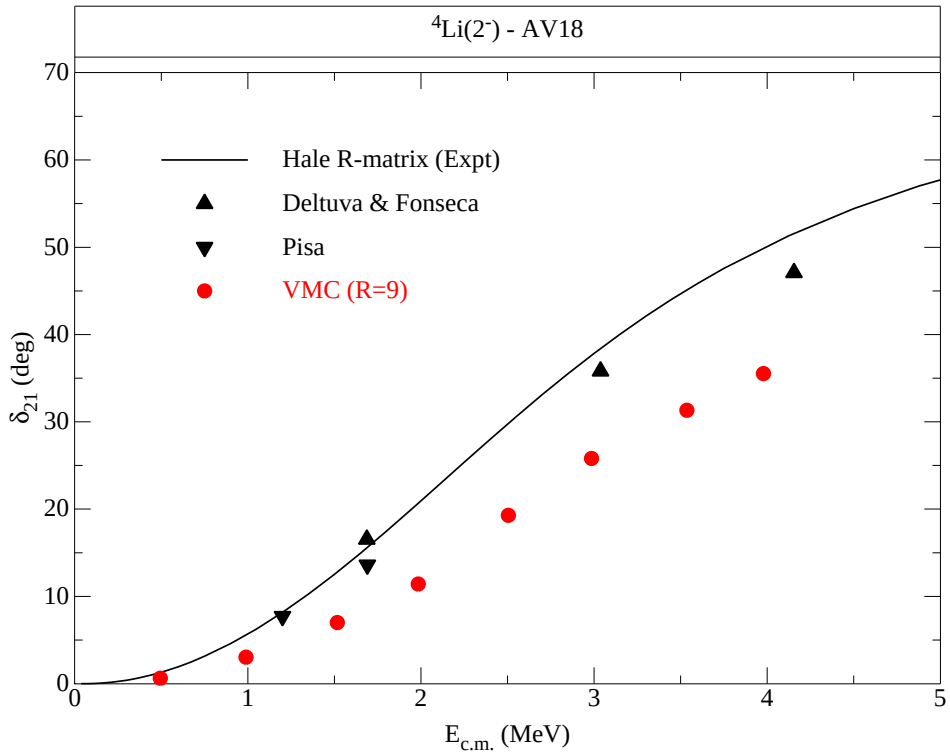
SCATTERING STATES IN ^{4}H AND ^{4}Li

- n–^{3}H and p–^{3}He provide incremental challenges to development of scattering capability
- Excellent few-body results from other groups like Lisbon & Pisa available for comparison
- Last year we had initial VMC results for single-channel n–^{3}H scattering
- First GFMC results for n–^{3}H and VMC for coupled-channels and p–^{3}He obtained this year

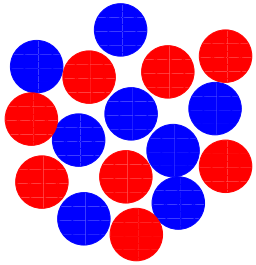


- Coupled channels look tricky, but Coulomb is no problem

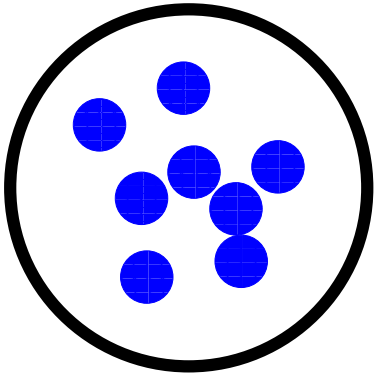




NEUTRON DROPS



NP self−bound



N confined

- Collection of neutrons interacting via standard NN and NNN Hamiltonian with added artificial external well $\sum_i V_{ext}(r_i)$
- Well can be adjusted to change density or surface thickness; may be non-spherical
- Realistic H can provide input to EDF's
- GFMC computed up to 16 neutrons (part-way through S–D shell).
- AFDMC computed beyond 50 neutrons

NEUTRON DROPS – WOODS-SAXON WELL

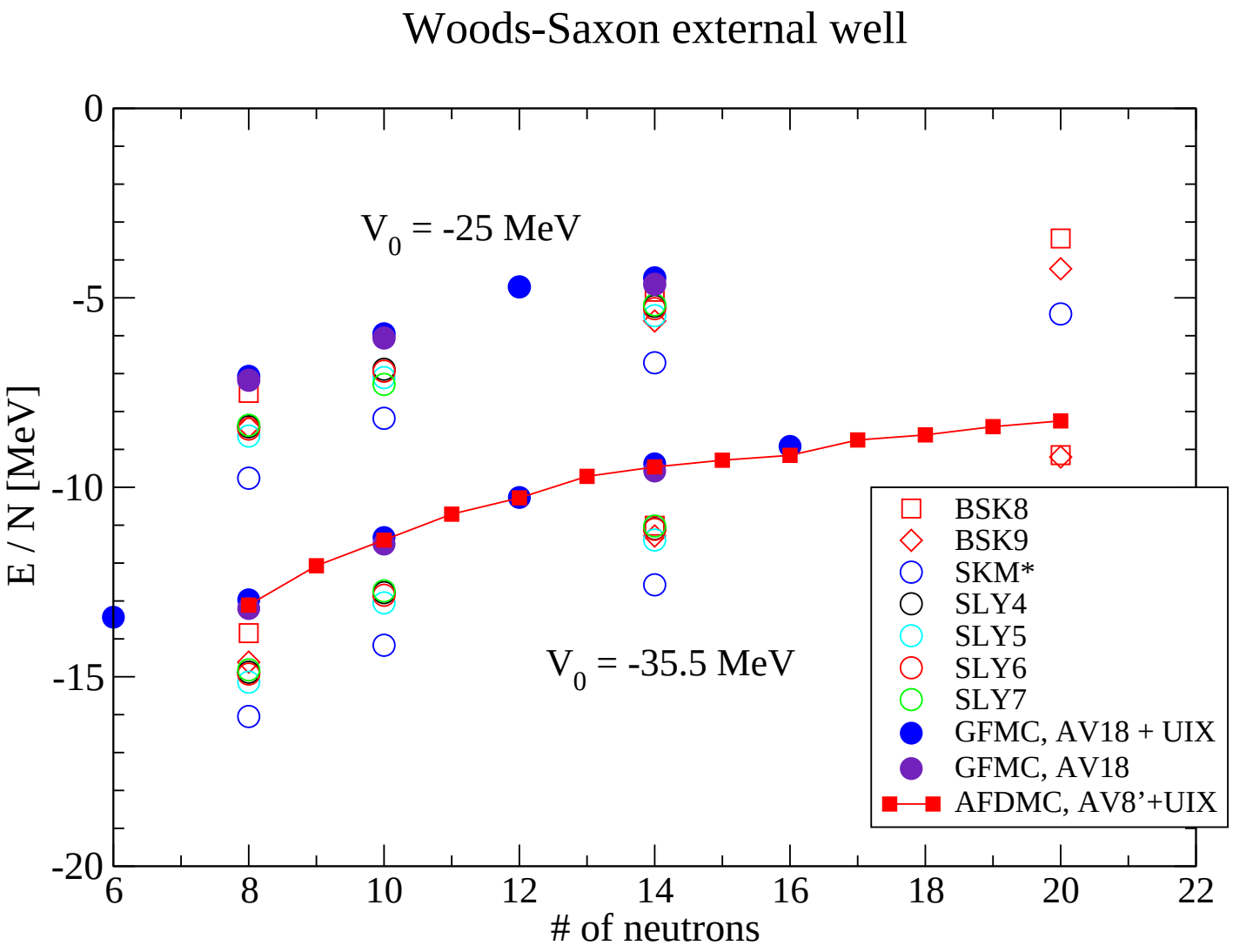
Comparison of GFMC and AFDMC energies.

Hamiltonian: AV8' + UIX + Wood-Saxon well, $V_0 = -35.5$ MeV, $R = 3$ MeV, $a = 1.1$

N	J^π	GFMC	AFDMC	% diff.
8	0^+	-103.9(1)	-104.9(1)	.9(1)
9	$1/2^+$	-107.8(1)	-108.6(1)	.8(1)
10	0^+	-113.4(1)	-113.9(1)	.4(2)
11	$5/2^+$	-116.9(2)	-117.8(2)	.8(2)
12	0^+	-123.6(3)	-123.4(2)	-.2(3)
13	$5/2^+$	-125.9(3)	-126.3(3)	.3(3)
14	0^+	-131.6(7)	-132.5(3)	.6(6)
16	0^+	-142.4(7)	-146.5(3)	2.8(5)

Agreement generally better than 1%.

Comparison of *ab-initio* and Skyrme models.



Skyrmes systematically overbind neutron drops.

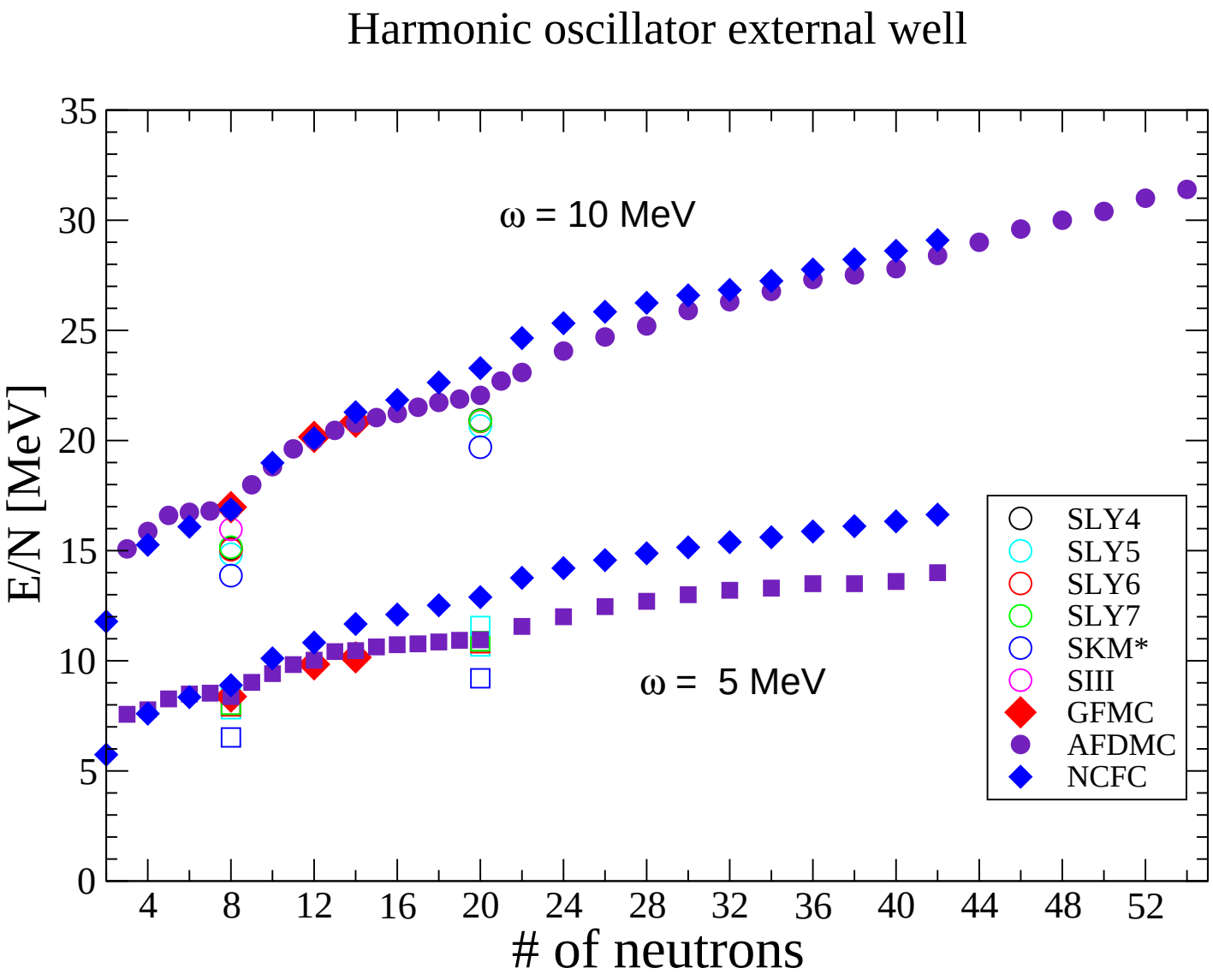
NEUTRON DROPS: HARMONIC OSCILLATOR WELL

Comparison of GFMC and AFDMC energies.
Hamiltonian: AV8' + UIX + Harmonic oscillator well

N	J^π	$\hbar\omega = 5MeV$			$\hbar\omega = 10MeV$		
		GFMC	AFDMC	% diff.	GFMC	AFDMC	% diff.
4	0^+	29.99(0)	31.1(1)	3.7(4)	62.04(1)	63.5(2)	2.4(3)
5	$3/2^-$	41.02(1)	41.8(3)	2.0(7)	82.97(1)	83.0(3)	.0(4)
5	$1/2^-$	41.22(1)	41.4(2)	1.0(2)	84.02(2)	83.6(3)	-.5(3)
6	0^+	48.52(1)	50.9(2)	5.0(3)	98.95(2)	100.4(3)	1.5(3)
7	$1/2^-$	59.17(1)	59.7(2)	1.0(4)	118.95(3)	117.7(4)	-1.1(3)
7	$3/2^-$	59.73(1)	60.3(2)	1.0(4)	121.08(3)	120.7(3)	-.3(2)
8	0^+	67.00(1)	67.0(2)	0.0(3)	135.80(4)	134.8(1)	-.7(1)
9	$1/2^+$	80.90(4)	81.2(1)	0.4(2)	163.7(1)	163.1(2)	-.4(2)
9	$5/2^+$	81.20(3)	81.6(2)	0.5(3)	163.2(1)	162.0(2)	-.8(1)
10	0^+	92.1(1)	94.2(2)	2.2(2)	188.2(5)	188.1(3)	-.0(1)
12	0^+	118.1(1)	120.3(3)	1.8(2)	242.0(6)	240.3(1)	-.7(2)
13	$5/2^+$	131.5(1)	135.4(3)	2.9(2)	267.6(6)	266.0(6)	-.6(3)
13	$1/2^+$	130.8(1)	135.9(3)	3.8(2)	268.0(5)	266.4(2)	-.6(2)
14	0^+	142.2(2)	146.4(3)	2.9(2)	291.9(2)	291.1(2)	-.3(1)

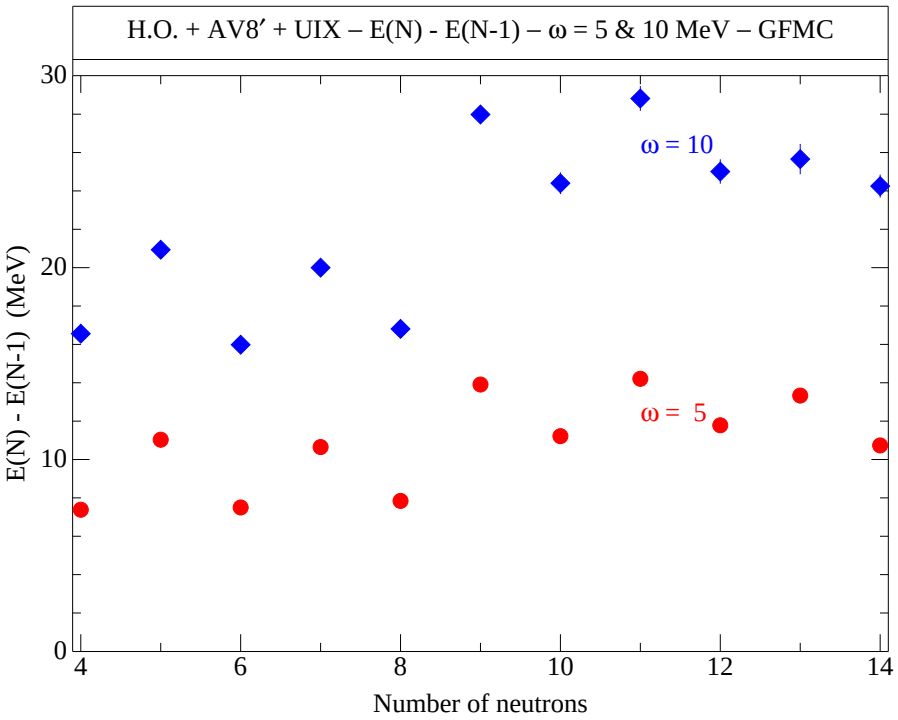
- $\hbar\omega = 5$ MeV, differences may be due to pairing effects (included in GFMC Ψ_V but not AFDMC)
- $\hbar\omega = 10$ MeV, agreement better than 1% except for smallest drops
- $3/2^- - 1/2^-$ and $5/2^+ - 1/2^+$ orderings reproduced in 6 of 8 cases

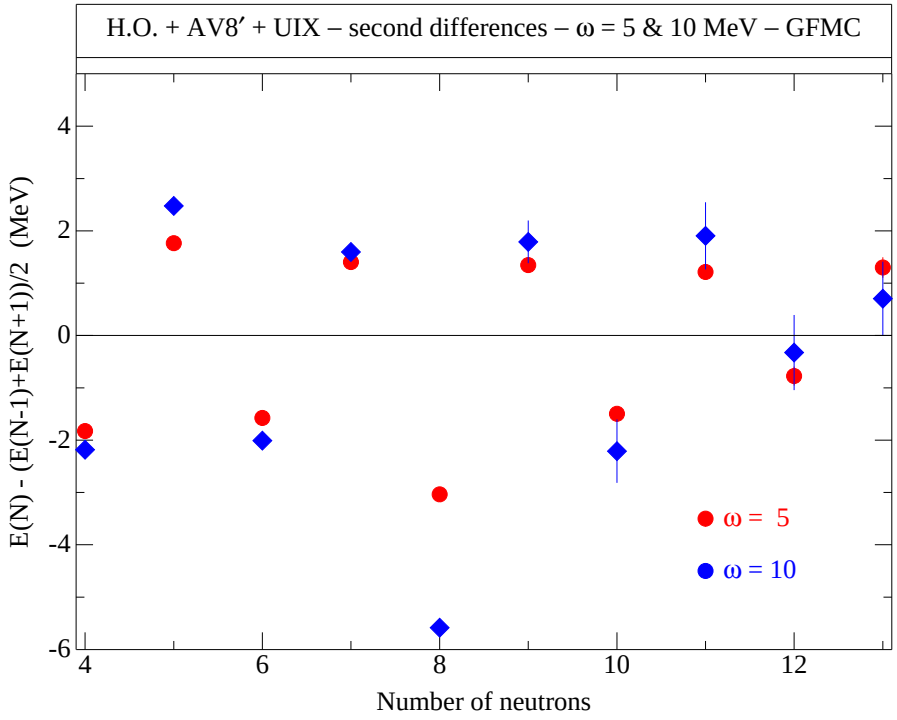
Comparison of *ab-initio* and Skyrme models.



NCFC (No Core Full Configuration) provided by P. Maris and J. Vary.

Even-odd staggering and pairing gap from GFMC.

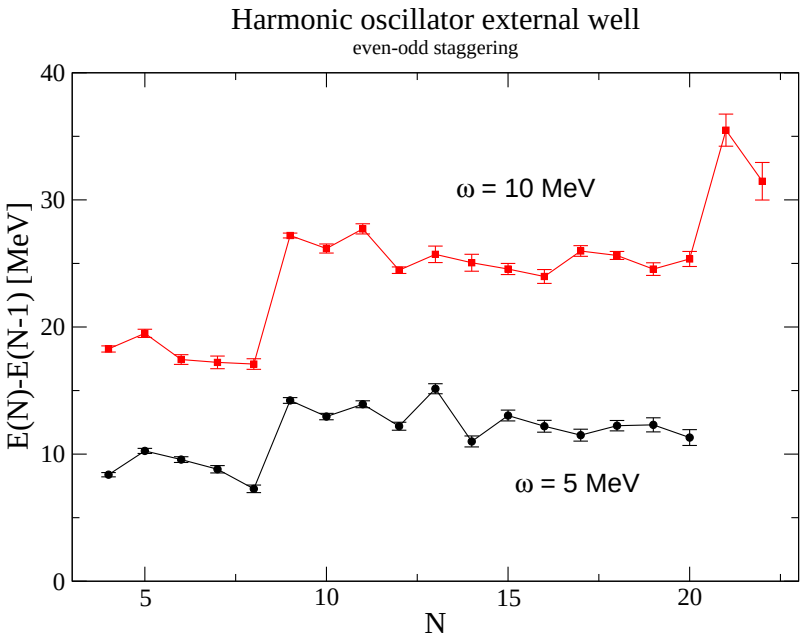




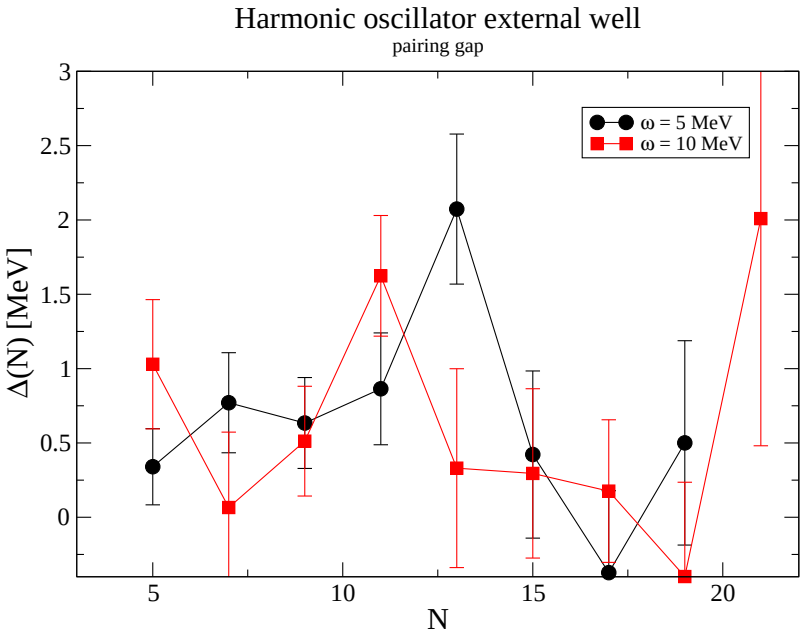
$$\Delta(N) = E(N) - E(N-1)$$

$$\Delta(N) = E(N) - \frac{E(N-1) + E(N+1)}{2}$$

Even-odd staggering and pairing gap from AFDMC.



$$\Delta(N) = E(N) - E(N-1)$$

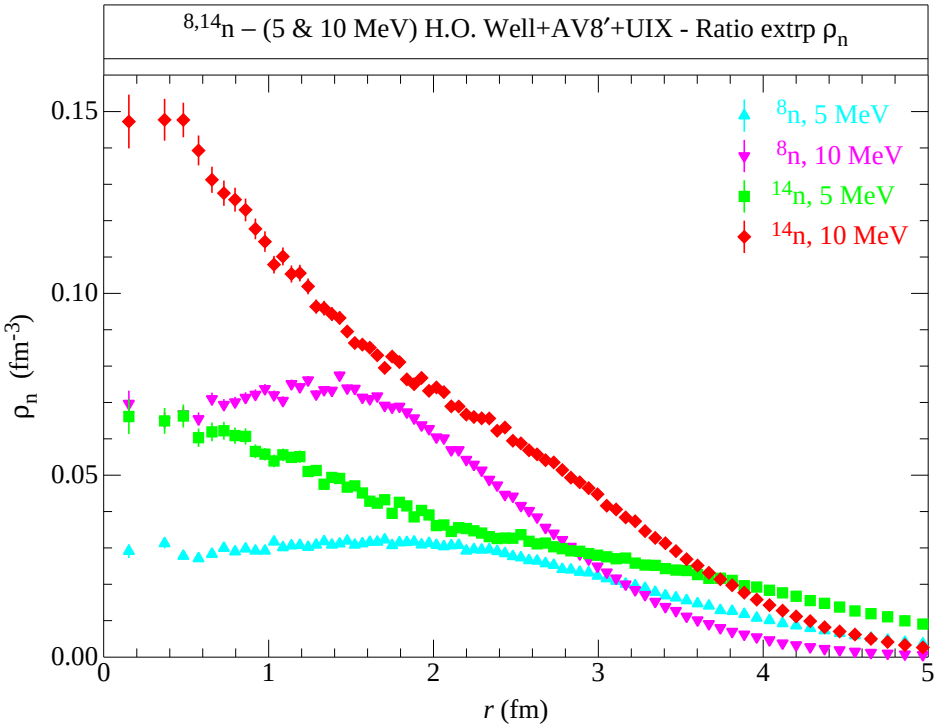


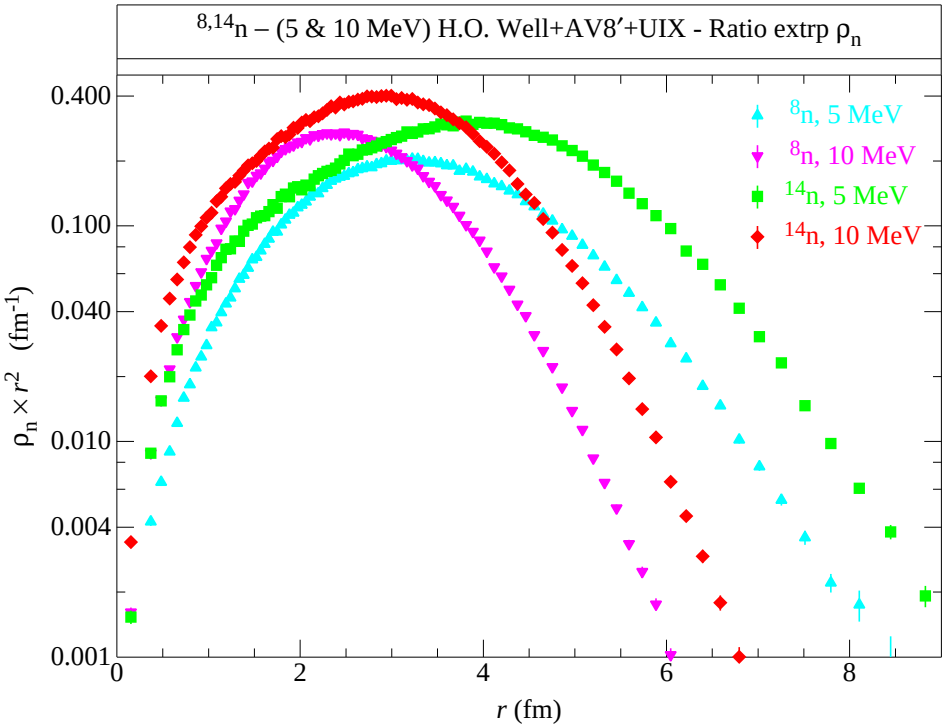
$$\Delta(N) = E(N) - \frac{E(N-1) + E(N+1)}{2}$$

Neutron Drops – Single-neutron Density Distributions

Oscillator well + AV18 + UIX

$\hbar\omega = 5\&10$ MeV





GFMC STUDY OF V_{ijk} CONTRIBUTIONS IN LIGHT NUCLEI

Calculations made for AV18+UIX plus additional terms in perturbation:

$$V_{ijk}^{2\pi} = A_{2\pi}^{PW}\Big(\sum_{cyc}\{X_{ij},X_{ik}\}\{\tau_i\cdot\tau_j,\tau_i\cdot\tau_k\} + \frac{1}{4}[X_{ij},X_{ik}][\tau_i\cdot\tau_j,\tau_i\cdot\tau_k]\Big)$$

$$X_{ij} = Y(m_\pi r_{ij})\sigma_i\cdot\sigma_j + T(m_\pi r_{ij})S_{ij}$$

$$V_{ijk}^{R} = A_R\sum_{cyc}T^2(m_\pi r_{ij})T^2(m_\pi r_{ik}) \;\;;\;\; V_{ijk}^{\pi R} = -A_R\sum_{cyc}T^2(m_\pi r_{ij})X_{ik}\tau_i\cdot\tau_k$$

Expectation values distributed over triples $\langle S'T|V_{ijk}|ST\rangle$

^{A}Z	S' S	unc	cor	$V^{2\pi A}$	$V^{2\pi C}$	$V^{2\pi S}$	V^{R}	$V^{\pi R}$
^{4}He	$\frac{1}{2}$ $\frac{1}{2}$	4	3.35	−2.35	−1.52	0.53	4.50	0.70
$T=\frac{1}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−5.01	−2.79	−1.02		4.52
	$\frac{3}{2}$ $\frac{3}{2}$		0.65	−0.02	−0.12	−0.04	0.91	0.00
total		4	4	−7.38	−4.43	−0.53	5.41	5.22
^{6}He	$\frac{1}{2}$ $\frac{1}{2}$	9.33	8.32	−2.51	−1.65	0.62	4.80	0.74
$T=\frac{1}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−5.72	−3.17	−1.19		5.04
	$\frac{3}{2}$ $\frac{3}{2}$	4	5.01	−0.00	−0.15	0.04	1.22	0.17
	$\frac{1}{2}$ $\frac{1}{2}$	6.67	6.12	0.05		0.02	0.25	0.02
$T=\frac{3}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−0.05		0.00		0.02
	$\frac{3}{2}$ $\frac{3}{2}$		0.55	−0.00		−0.00	0.15	0.00
total		20	20	−8.23	−4.97	−0.51	6.28	5.99

^{A}Z	S' S	unc	cor	$V^{2\pi A}$	$V^{2\pi C}$	$V^{2\pi S}$	V^R	$V^{\pi R}$
^{8}He	$\frac{1}{2}$ $\frac{1}{2}$	17.33	15.67	−2.85	−1.89	0.75	5.55	0.81
T=$\frac{1}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−7.28	−3.90	−1.58		6.22
	$\frac{3}{2}$ $\frac{3}{2}$	10.67	12.33	−0.05	−0.25	0.16	1.88	0.52
	$\frac{1}{2}$ $\frac{1}{2}$	22.67	20.72	0.07		0.05	0.81	0.06
T=$\frac{3}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−0.16		−0.00		0.08
	$\frac{3}{2}$ $\frac{3}{2}$	5.33	7.28	0.03		−0.01	0.08	0.00
total		56	56	−10.24	−6.04	−0.62	8.32	7.69
^{8}Be	$\frac{1}{2}$ $\frac{1}{2}$	24	21.75	−5.02	−3.30	1.20	9.70	1.48
T=$\frac{1}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−11.14	−6.18	−2.24		10.03
	$\frac{3}{2}$ $\frac{3}{2}$	16	18.25	0.02	−0.31	0.00	2.33	0.25
	$\frac{1}{2}$ $\frac{1}{2}$	16	14.12	0.11		0.04	0.26	0.02
T=$\frac{3}{2}$	$\frac{1}{2}$ $\frac{3}{2}$			−0.06		0.00		0.03
	$\frac{3}{2}$ $\frac{3}{2}$		1.88	−0.00		−0.00	0.02	0.00
total		56	56	−16.09	−9.79	−1.00	12.31	11.81

Observations:

- ∼2/3 of $\langle V^{2\pi P}\rangle$ comes from coupling $S'S$ = $\frac{1}{2}$ $\frac{3}{2}$ components (requires D-state components in Ψ)
- T=$\frac{3}{2}$triples contribute nothing to $\langle V^{2\pi P}\rangle$
- $\langle V^{2\pi S}\rangle$ is $< 5\%$ of $\langle V^{2\pi P}\rangle$
- $\langle V^R\rangle$ is diagonal in $S'S$ while $\langle V^{\pi R}\rangle$ is mostly off-diagonal; however they scale the same with A,Z

STATUS OF DELIVERABLES FOR THIS YEAR

- Calculate ab initio one-body densities for spherical and deformed nuclei and use them to inform DFT
  – Done for spherical drops in several harmonic oscillator wells
- Calculate lowest 2^+ excitation and $E2$ transition form factor for ^{12}C with GFMC
  – Not yet done; postponed to next year
- Initial work toward ^{12}C(0_2^+) Hoyle State
  – Lots of attempts made; some good VMC results, but no good GFMC result so far
- Improve Asynchronous Dynamic Load-Balancing for largest computers
  – Very good scaling to 131,072 cores achieved
- Ab-initio calculations for deformed and superfluid neutron drops in external potentials with comparisons to DFT
  – GFMC for N=3–16 in h.o. well; comparisons with AFDMC show good agreement;
  – AFDMC calculations beyond N=50; new Skyrme models being made
- Investigate reactions in light nuclei using ab initio methods: NCSM with RGM, GFMC, and J-matrix methods. Benchmark n-7Li, n-8He, and n-9Li scattering
  – n–^{3}H & p–^{3}He scattering being done in VMC & GFMC

Following should have been in the list

- GFMC calculations of nuclear overlaps and spectroscopic factors
  – Being done now for $\langle ^3\mathrm{H}+p\,|^4\mathrm{He}\rangle$, $\langle ^6\mathrm{Li}+n\,|^7\mathrm{Li}\rangle$, and $\langle ^6\mathrm{He}+p\,|^7\mathrm{Li}\rangle$ – see Brida's talk

PLANS

Remainder of this year

- Continue ADLB work aimed at next generation machines
- Continue work on ^{12}C(0_2^+) Hoyle state
- Deformed neutron-drop calculations if desired
- GFMC nuclear overlaps $\langle (A-1)+N\,|A\rangle$ up to A=10
- GFMC n–^{3}H & p–^{3}He scattering including coupled channels

Year 5

- Continuing ADLB work in GFMC – finer-grain parallelization for next generation machines
- More ^{12}C calculations, including 2^+ state and $E2$ transition
- GFMC n–^{7}Li & α–α scattering
- Start GFMC $\langle (A-2)+NN\,|A\rangle$, etc. overlaps
- VMC (GFMC?) computation of density matrix if interesting