GFMC Calculations of Carbon

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Partners in crime

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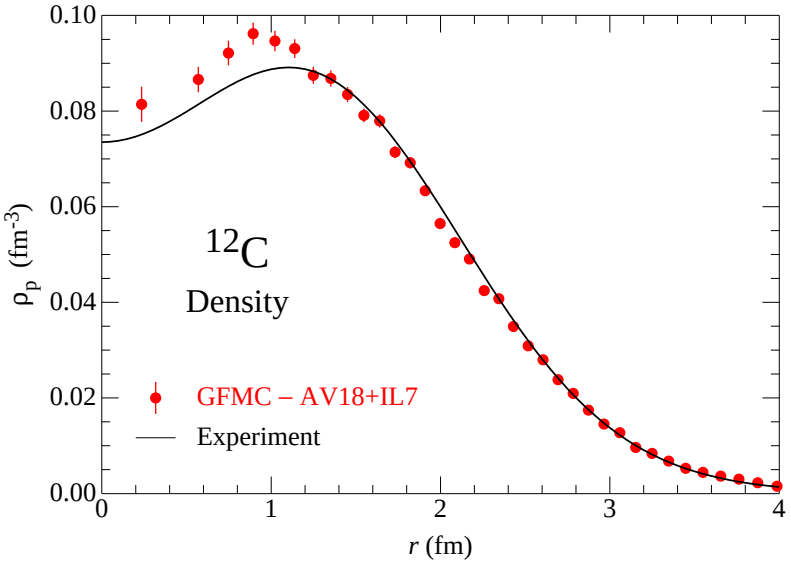

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Exploring Nuclear Matter - Quarks to Stars

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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

v_{ij}: Argonne v18 (1995)

$$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R} + v_{ij}^{CIB}$$

v_{ij}^{γ}: pp, pn & nn electromagnetic terms, Coulomb, magnetic, etc. with form factors

v_{ij}^{π} $[Y(r_{ij})\sigma_i \ \ \sigma_j + T(r_{ij})S_{ij}] \ \ \tau_i \ \ \tau_j$; $\langle v_{ij}^{\pi} \rangle$ contributes 85% of $\langle v_{ij} \rangle$

$v_{ij}^{R} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^{p}$

$O_{ij}^{p=1,14} = [1, \sigma_i \ \ \sigma_j, S_{ij}, \mathbf{L} \ \ \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2\sigma_i \ \ \sigma_j, (\mathbf{L} \ \ \mathbf{S})^2] \ \ [1, \tau_i \ \ \tau_j]$

Determined phenomenologically

v_{ij}^{CIB}: 4 operators for nuclear charge independence breaking

AV18 is a direct fit to the Nijmegen data base:

1787 pp, 2514 pn, 1 nn data for $E_{Lab} < 350$ MeV 40 parameters; χ^2/d.o.f. = 1.09

Typical of 1990's NN potentials

R.B. Wiringa, V.G.J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, (1995)

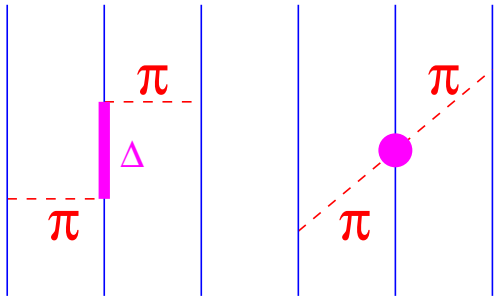
NUCLEAR HAMILTONIAN – ILLINOIS V_{ijk}

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

$V_{ijk}^{2\pi}$: Fujita-Miyazawa + s-wave term; in most V_{ijk}

Longest ranged V_{ijk}

Attractive in all nuclei studied.



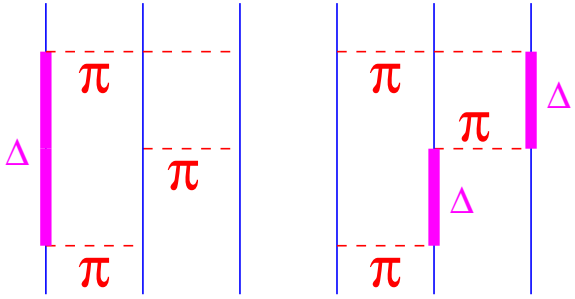
$V_{ijk}^{3\pi}$: 3π rings with 's; new in Illinois V_{ijk}

Extra p-shell, jN Zj attraction

One in energy denominator

2 , 3 denominators not yet considered

$hV_{ijk}^{3\pi}i < 0.1hV_{ijk}^{2\pi}i$



V_{ijk}^{R}: represents all else including relativistic effects – purely central and repulsive

3-4 Couplings adjusted to fit 17 nuclear levels for A 8

In light nuclei we find $hV_{ijk}i$ (0.02 to 0.09)$hv_{ij}i$ (0.15 to 0.6)hHi

(Large cancellation of K and v_{ij})

We expect $hV_{4N}i$ 0.06$hV_{ijk}i$ (0.02 to 0.04)hHi (0.5 to 2.) MeV

But not possible to disentangle from V_{ijk} uncertainties.

S.C. Pieper, V.R. Pandharipande, R.B. Wiringa, and J. Carlson, Phys. Rev. C **64**, 014001 (2001)

Pieper, AIP CP **1011**, 143 (2008)

THE MANY-BODY PROBLEM

Need to solve

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

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

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

$2^A \quad \binom{A}{Z}$ complex coupled 2^{nd} order eqn in $3A$ variables

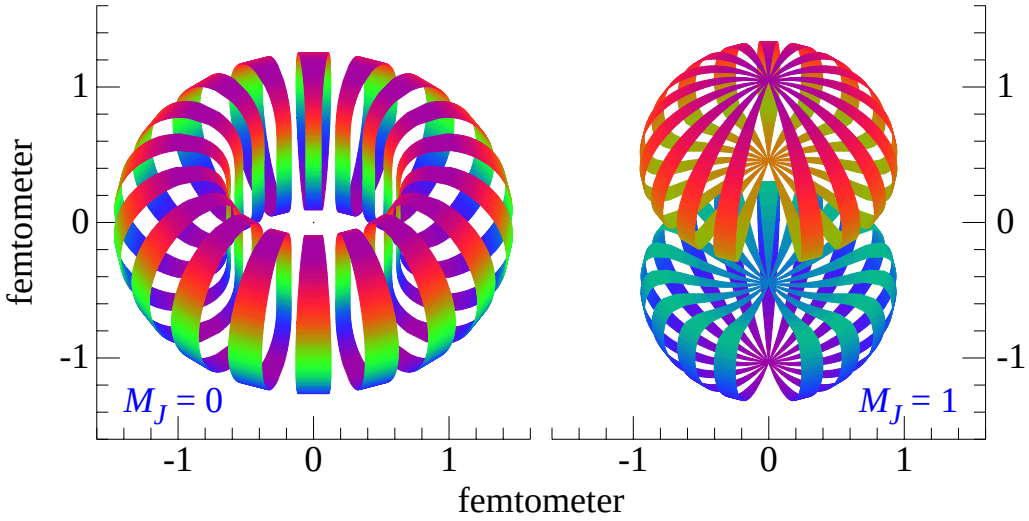
(number of isospin states can be reduced)

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

Coupling is strong:

$\langle v_{\text{Tensor}} \rangle$ is 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

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \qquad E_0$$

Monte Carlo integration (Metropolis random walk) is used for the $3A$-dimensional integral

Simplified trial wave function:

$$|\Psi_T\rangle = \mathcal{S} \prod_{i<j} \left[1 + U_{ij} + \sum_k U_{ijk} \right] \prod_{i<j} f_{ij} |\Phi\rangle$$

is a fully antisymmetric combination of one-body wave functions $\phi_i(\vec{r_j})$

determines quantum numbers of state

translationally invariant – written in terms of $\vec{r_i} \qquad \vec{R_{\rm cm}}$

has multiple spatial-symmetry components; usually in LS basis

Can be made with arbitrary $\phi_i(\vec{r_j})$,

e.g. solutions, with correct asymptotic behavior, of Woods Saxon potentials

Can have sub-cluster structure, like α+t+n for ^{8}Li or α+α+α for ^{12}C

f_{ij} are central (mostly short-ranged repulsion) correlations

U_{ij} are non-commuting 2-body correlations from v_{ij}

U_{ijk} are 3-body correlations from V_{ijk}

GREEN'S FUNCTION (DIFFUSION) MONTE CARLO

VMC $_T$ propagated to imaginary time τ:

$$(\tau) = e^{(H \quad E_0)\tau} \quad _T$$

$$_T = \quad _0 + \sum \alpha_i \quad _i \quad ; \qquad (\tau) = e^{(E_0 \quad E_0)\tau} \quad [\quad _0 + \sum \alpha_i e^{(E_i \quad E_0)\tau} \quad _i]$$

$$_0 = \lim_{\tau \,!\, 1} \quad (\tau) \quad ; \quad H \quad _0 = E_0 \quad _0$$

Small imaginary-time-step propagator:

$$(\tau) = \left[e^{(H \quad E_0)\,4\,\tau}\right]^n \quad _T; \quad \tau = n\,4\,\tau$$

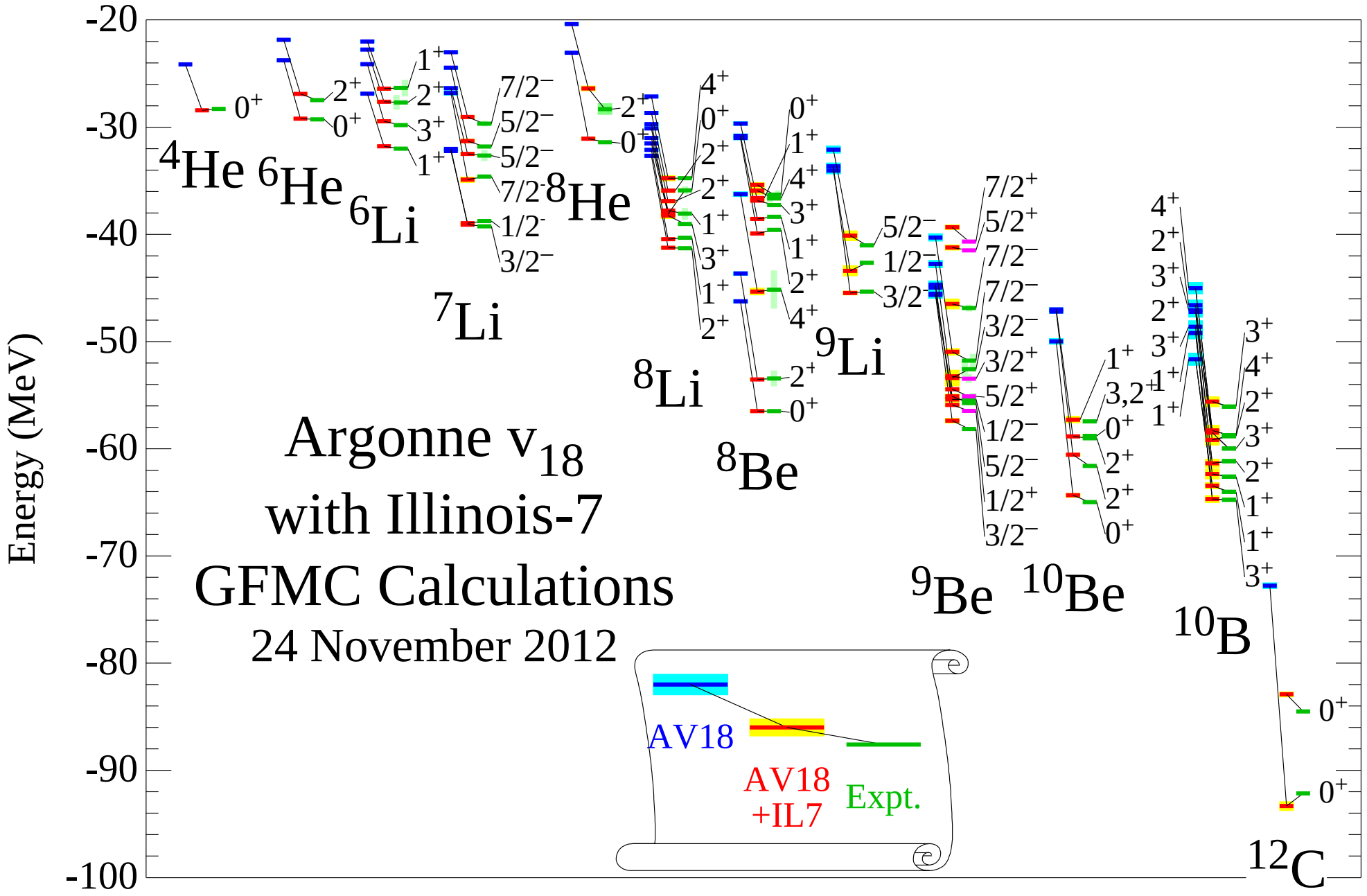
Can be computed to order $(4\tau)^3$

$$G_{\beta\alpha}(\mathbf{R}^0, \mathbf{R}) = h\mathbf{R}^0, \beta j e^{(H \quad E_0)\,4\,\tau} j\mathbf{R}, \alpha i$$

$$(\mathbf{R}_n, \tau) = \int G(\mathbf{R}_n, \mathbf{R}_{n \quad 1}) \quad G(\mathbf{R}_1, \mathbf{R}_0) \quad _T(\mathbf{R}_0) d\mathbf{R}_{n \quad 1} \quad d\mathbf{R}_0$$

$$E(\tau) = \frac{h \quad _T j H j \quad (\tau) i}{h \quad _T j \quad (\tau) i} \quad E_0$$

Done by Monte Carlo integration – $3An$ dimensions (typically 36,000 for ^{12}C)


Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
Argonne v18
with Illinois-7
GFMC Calculations
24 November 2012
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C
AV18
AV18
+IL7
Expt.

MIRA – ARGONNE'S IBM BLUE GENE Q

48 racks of nodes
1024 nodes per rack: 49,152 nodes
16 Gbytes memory per node: 768 Tbytes
16 cores per node: 786,432 cores
4 threads per core: 3,145,728 threads
1.6 GHz clock; 4 multiply-add per cycle
12.8 GFLOP/core: 205 GFLOP per node,
10 PFLOP
5-D torus network: 1.8 GByte/s bandwidth

19.6 Pbytes (22 10^{15}) disk
Filesystem 1K-blocks ...
/dev/mira-fs0 20406463365120 ...
240 Gbyte/sec bandwidth
80 watt/node: 3.9 Mwatt for nodes
2.5 GFLOP per watt
water cooled - 20–30 gpm per rack:
1,000 gpm for nodes

1/3 of Mira – one row (16 racks) of three

OpenMP Strong Scaling

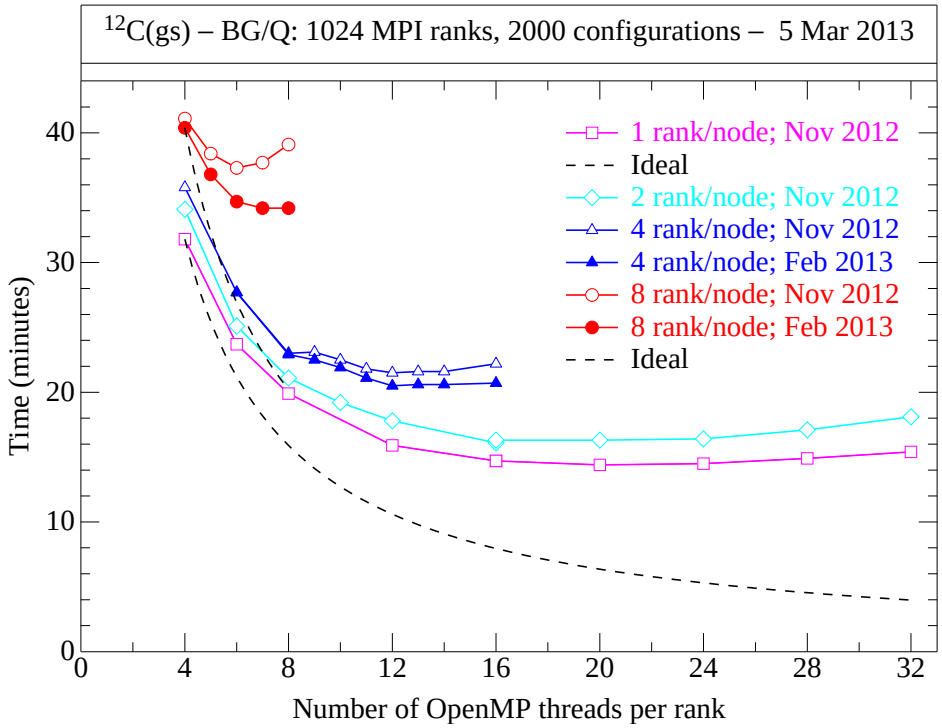
$^{12}C(0^+)$ – 2000 configs for 40 time steps (2 energies) on 1024 ranks

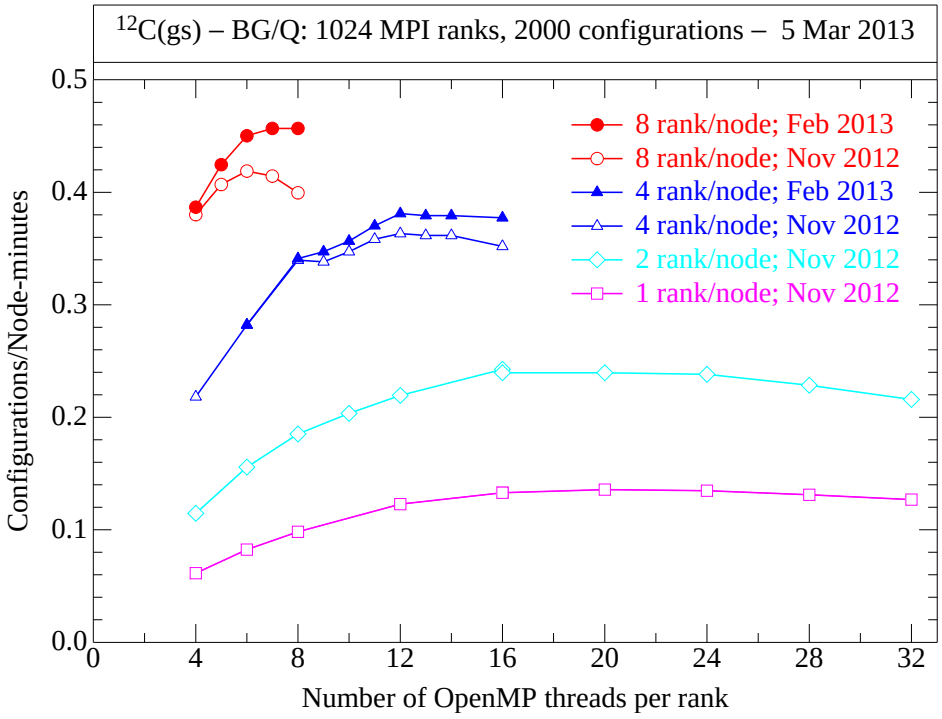
Time increases as with more ranks/node

Optimal speed obtained with fewer than max. possible threads

– Memory contention

Best overall use of nodes obtained with most ranks/node





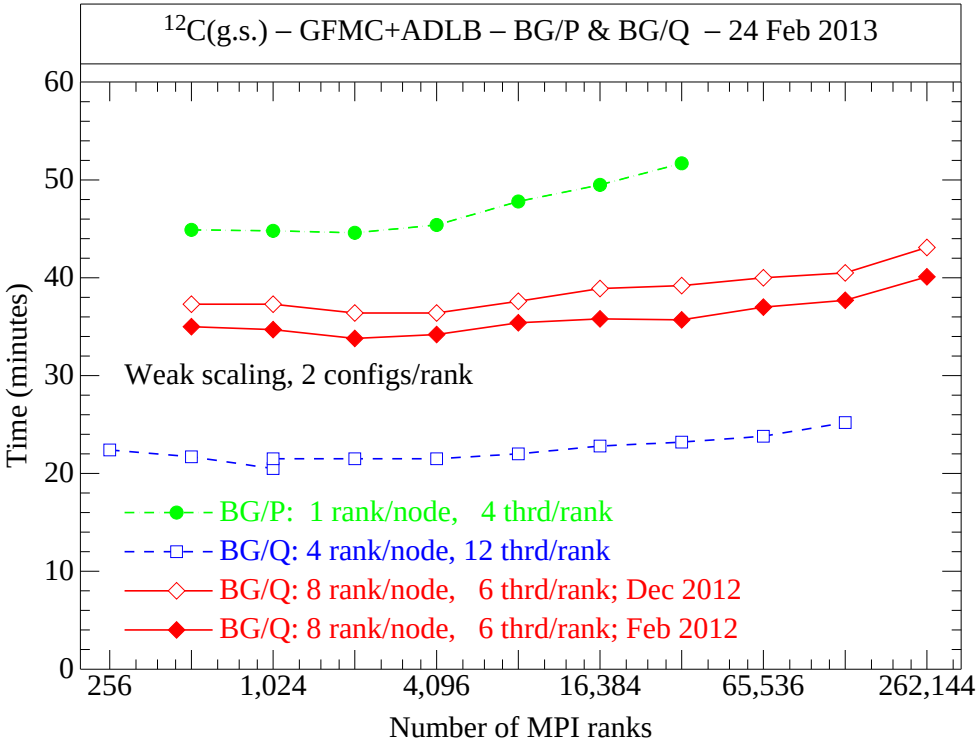
ADLB Weak Scaling

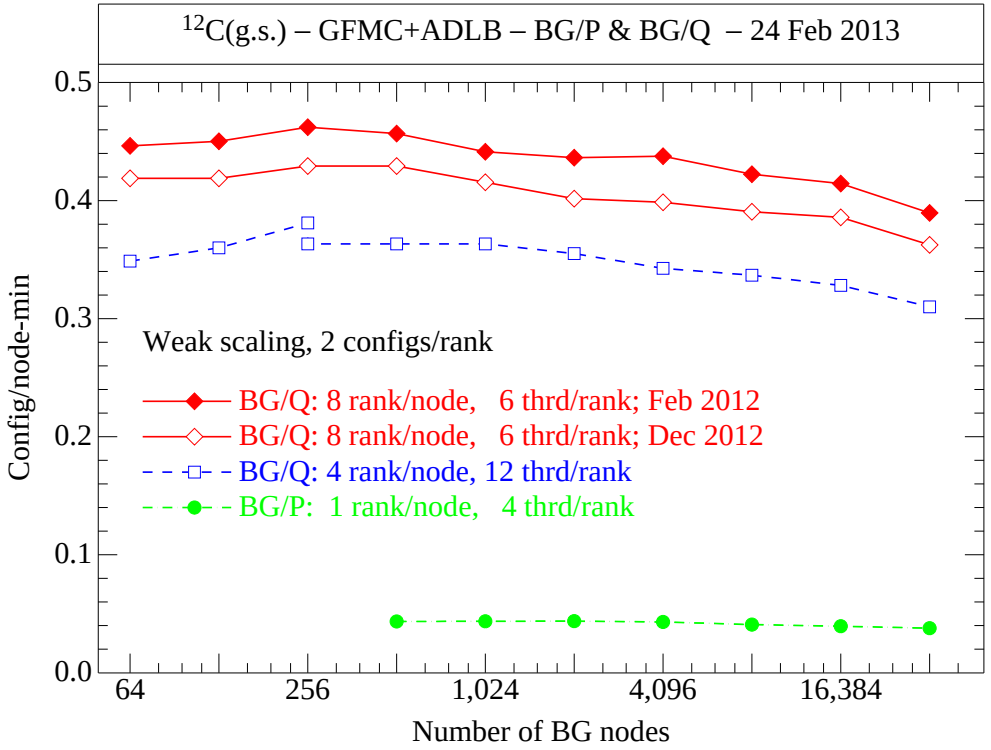
$^{12}C(0^+)$ – 2 configs/rank for 40 time steps (2 energies)

Best overall use of nodes obtained with most ranks/node

Good scaling to 262,000 ranks – 524,288 cores – 1,572,864 threads!

BG/Q node performance 10 BG/P node





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

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

There are 5 LS-basis J=0^+ states in ^{12}C: ^{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. For example

$$^3\mathrm{P}_0[4431] \quad = \quad \frac{1}{4\ \ 32}\Big\{8\ \ 27\ \ 13 + 26\left(24 + \sum_{i<j}\boldsymbol{\sigma}_i\ \ \boldsymbol{\sigma}_j\right)\sum_{i<j}\boldsymbol{\sigma}_i\ \ \boldsymbol{\sigma}_j$$

$$+\left[4\ \ 27 + \left(24 + \sum_{i<j}\boldsymbol{\sigma}_i\ \ \boldsymbol{\sigma}_j\right)\sum_{i<j}\boldsymbol{\sigma}_i\ \ \boldsymbol{\sigma}_j\right]\sum_{i<j}\boldsymbol{\sigma}_i\ \ \boldsymbol{\sigma}_j\boldsymbol{\tau}_i\ \ \boldsymbol{\tau}_j\Big\}\quad [(p_{3/2})^8]$$

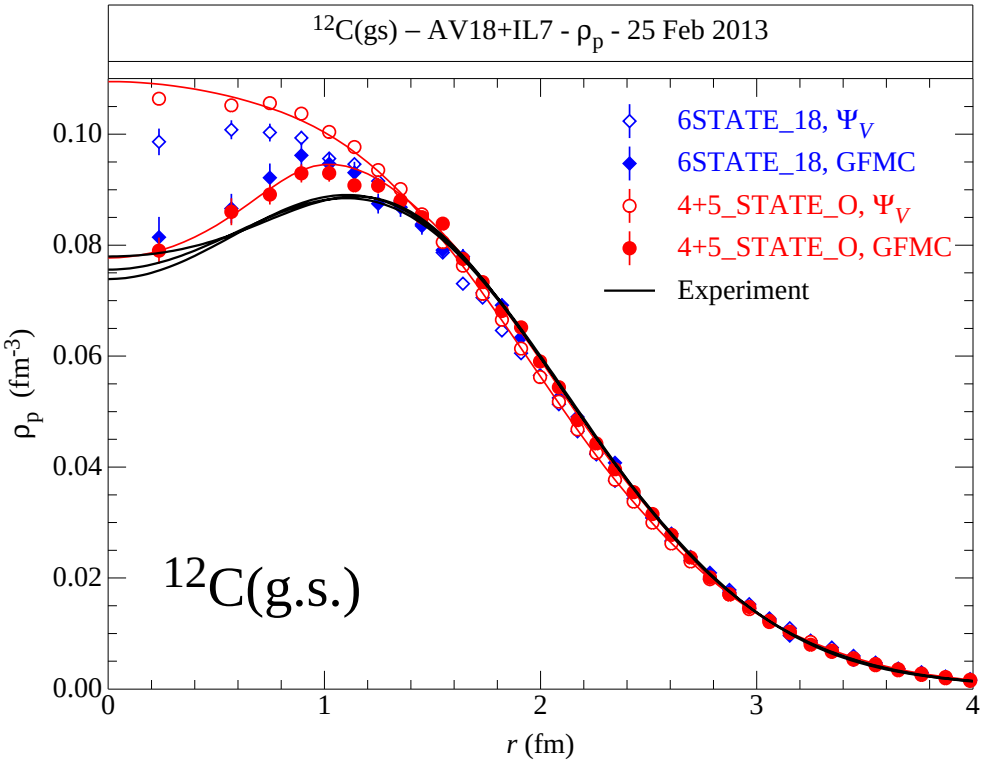
^{12}C states have strong triple-alpha structure; Pandharipande made a subroutine that explicitly makes triple-alpha states with one α in the $0S$ shell and two in the $0P$ shell.

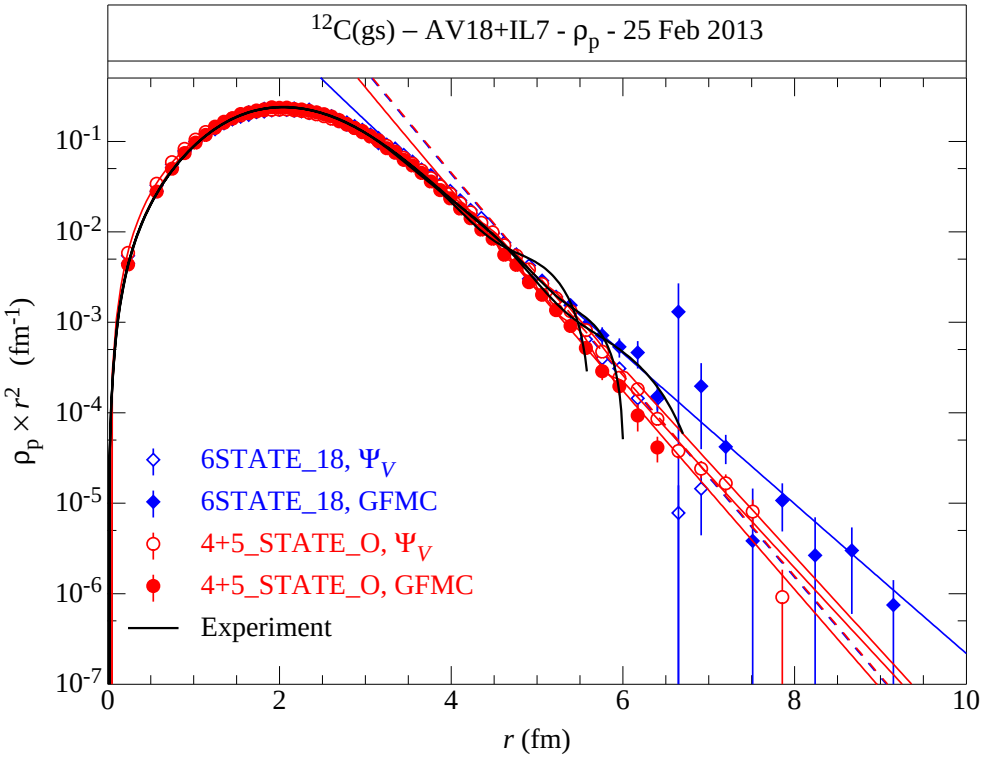
We consider all 6 states and find ground-state contributions like

3-α	^{1}S[444]	^{3}P[4431]	^{1}S[4422]	^{5}D[4422]	^{3}P[4332]
84.%	3.%	13.%	0.19%	0.28%	0.18%
43.%	42.%	14.%	0.015%	0.39%	0.10%

The 3-α & ^{1}S[444] states can be very degenerate.

^{12}C(G.S.) RESULTS ONE-BODY DENSITY





The T density is significantly improved by GFMC

Central dip is generated

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

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 3α ! ^{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 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 $0P^2 1S^2$

Total of 11 states to be diagonalized in v

The $1S$-$0D$ shell one-body $\phi(r)$ are given a large RMS radius

Suggestion of Kevin Schmidt:

We make an initial diagonalization to get the g.s. v

Then compute overlaps of the GFMC g.s. propagation with the 11 components of v

Diagonalize these overlaps (rank 10) to get the next 0^+ state

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

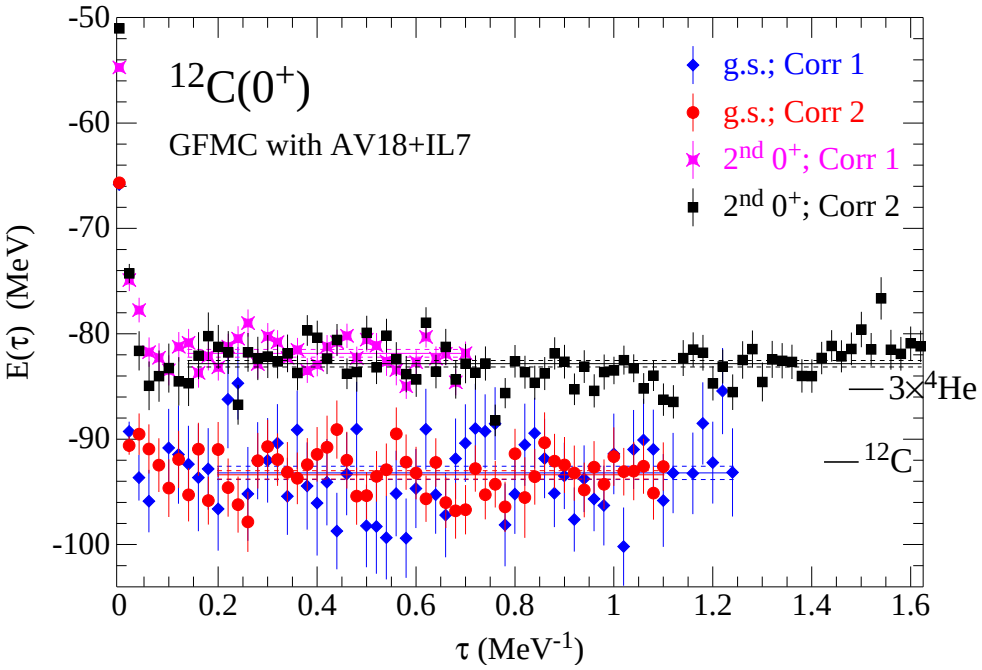
One example of the diagonalization

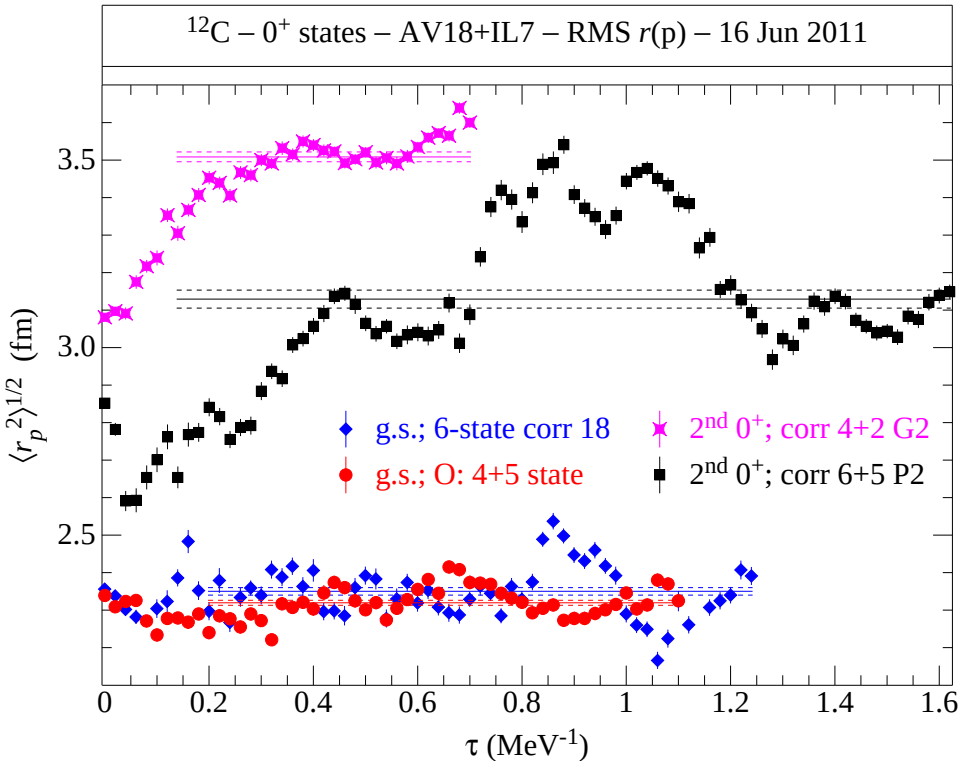
	3-α states				LS P-shell states				
	$0P^4$	$0D^4$	$1S^4$	$0D^2 1S^2$	^{1}S[444]	^{3}P[4431]	^{1}S[4422]	^{5}D[4422]	^{3}P[4332]
gs	43.%	0.0%	0.0%	0.6%	42.%	14.%	0.015%	0.39%	0.10%
2^{nd} 0^+	12.%	62. %	1.0%	5.6%	18.%	1.5%	0.13%	0.0%	0.05%

Shells of the last α are shown

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

^{12}C Convergence as a function of imaginary time (τ)

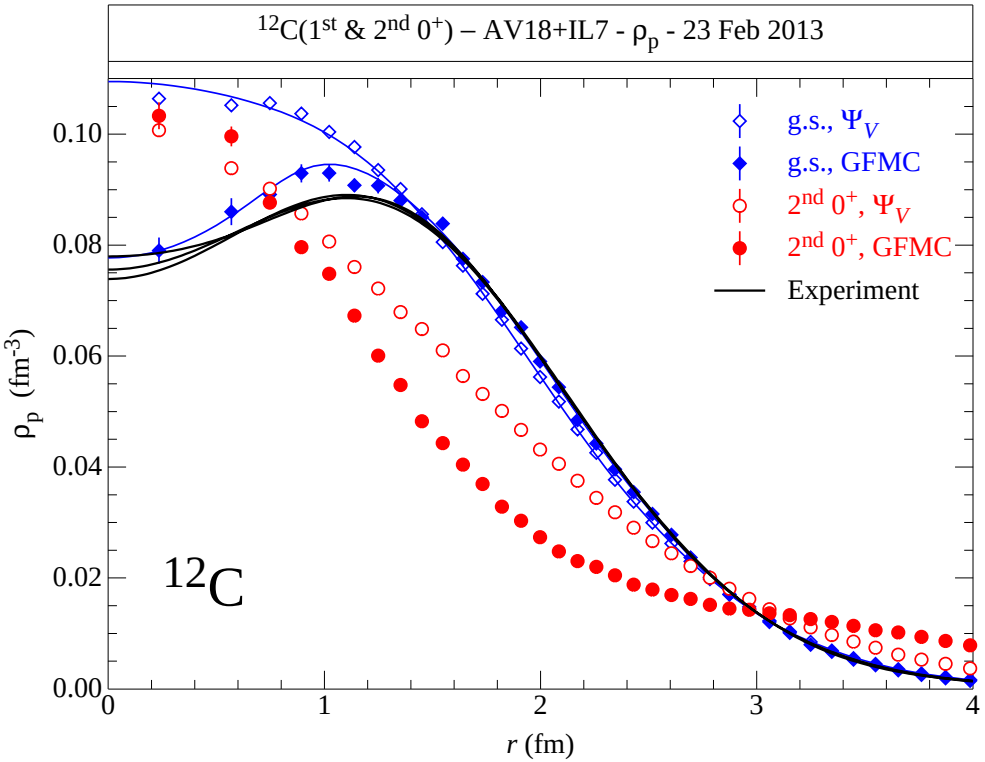


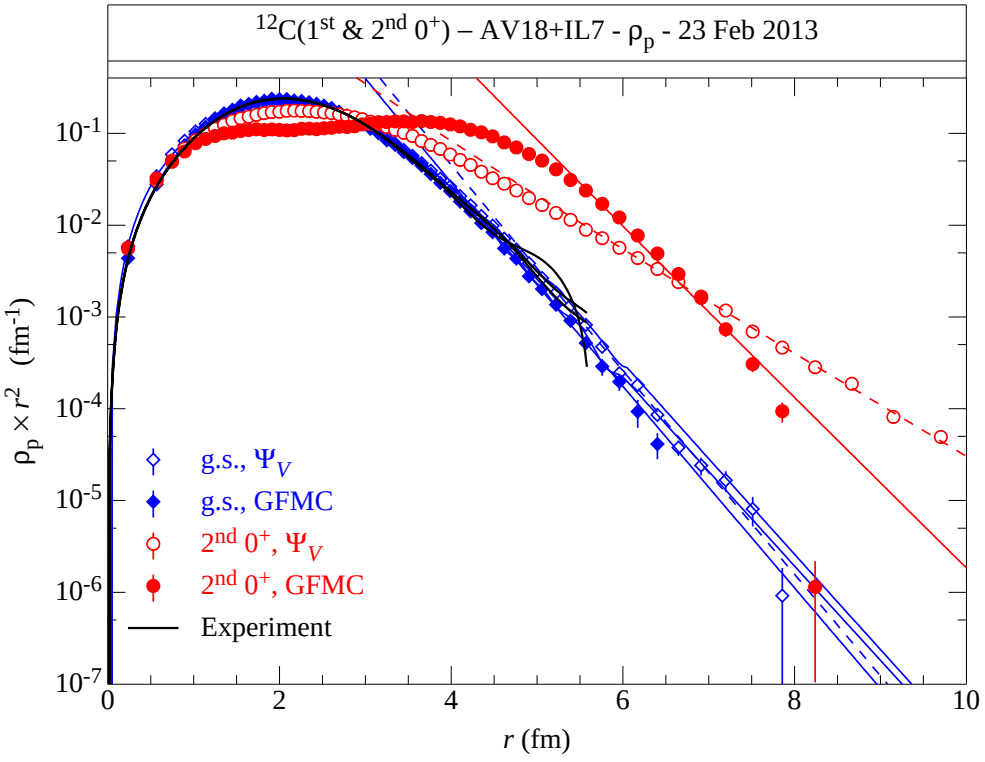


	g.s. energy			2^{nd} 0^+ E		
	VMC	GFMC	Expt.	VMC	GFMC	Expt.
AV18	–44.9(2)	–73.2(5)		10.0(3)	7.9(6)	
AV18+IL7	–65.7(2)	–93.3(4)	–92.16	14.7(2)	10.4(5)	7.65

^{12}C – 1^{st} & 2^{nd} 0^+ States

One-body density



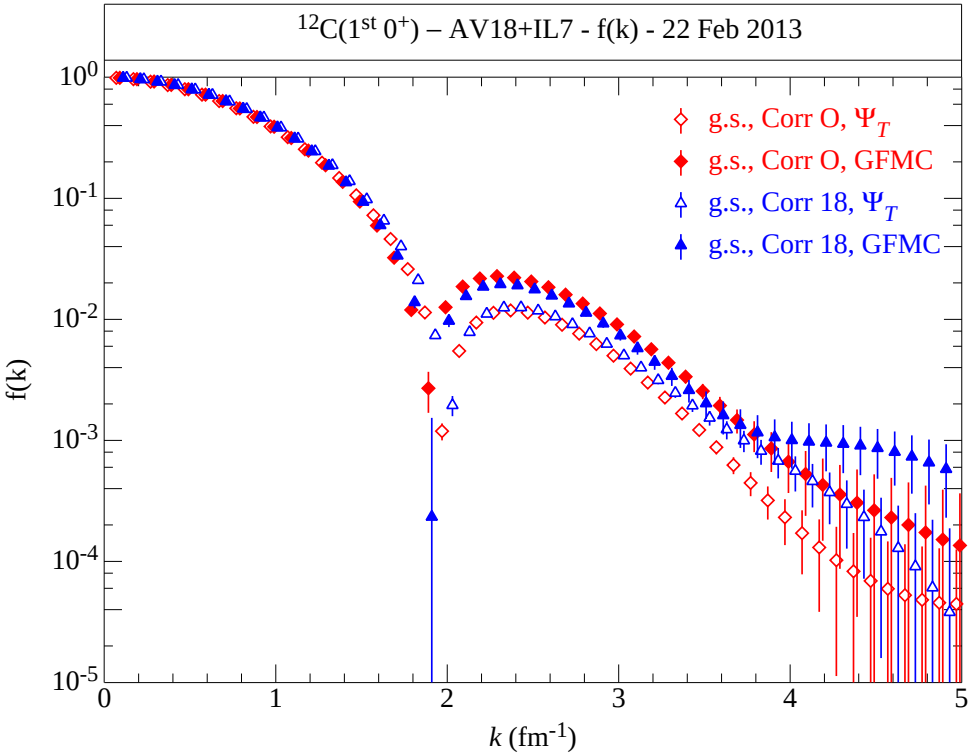


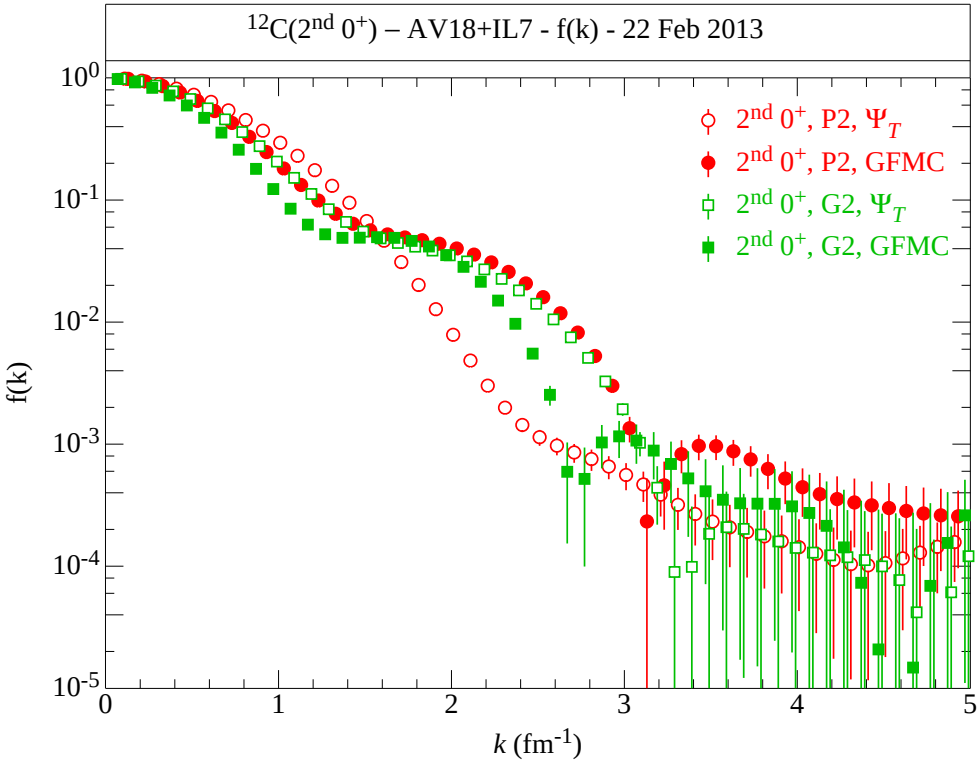
Ground-state $\rho(r)$ has dip at $r = 0$ – suggests equilateral triangle of 3 α's

2^{nd} 0^+ $\rho(r)$ has no dip at $r = 0$ – suggests line of 3 α's

^{12}C – 1^{st} & 2^{nd} 0^+ States

Form factor





GFMC g.s. form factors from different T agree well to 4 fm [1]

Not the case for the 0_2^+ state

^{12}C(G.S.) ! ^{12}C(0_2^+) $E0$ FORM FACTOR

Radiative decay rate of Hoyle state important for astrophysics

Measurements over last 50 years of $E0$ excitation.

Recent reanalysis of world data in
M. Chernykh *et al.*, Phys. Rev. Lett. **105**, 022501 (2010)

Strongest known $E0$ to single state; 7.5% of energy-weighted sum rule

$M(E0)$ $h0_2^+ jr^2 P_p j$g.s.i; P_p is proton projector

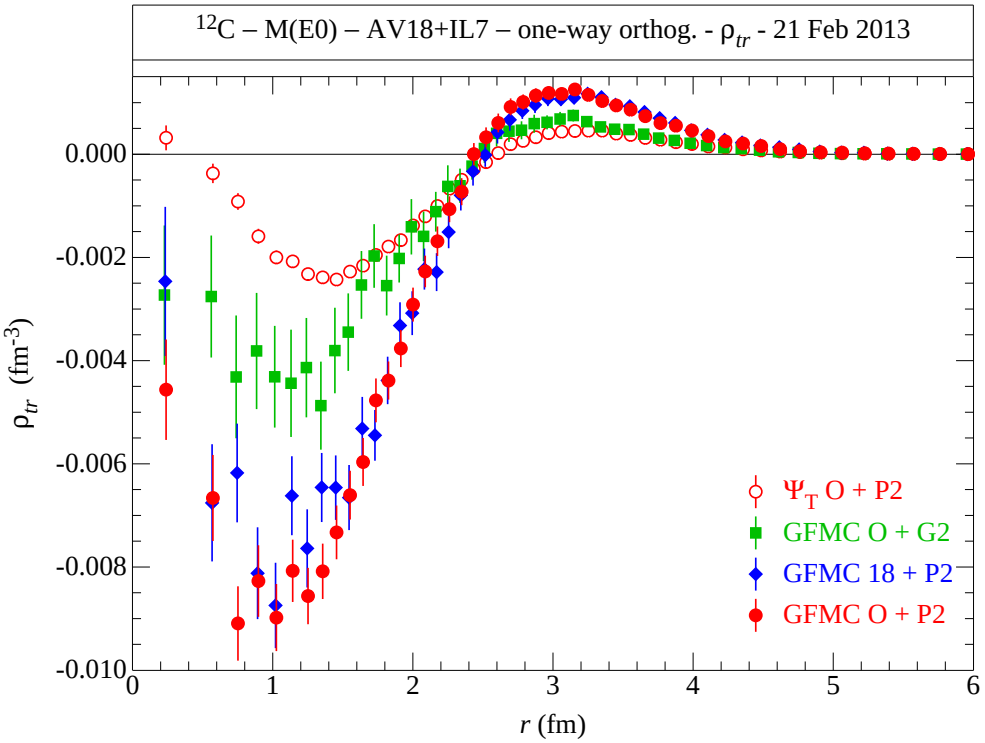
remember $h0_2^+ j$g.s.$i = 0$

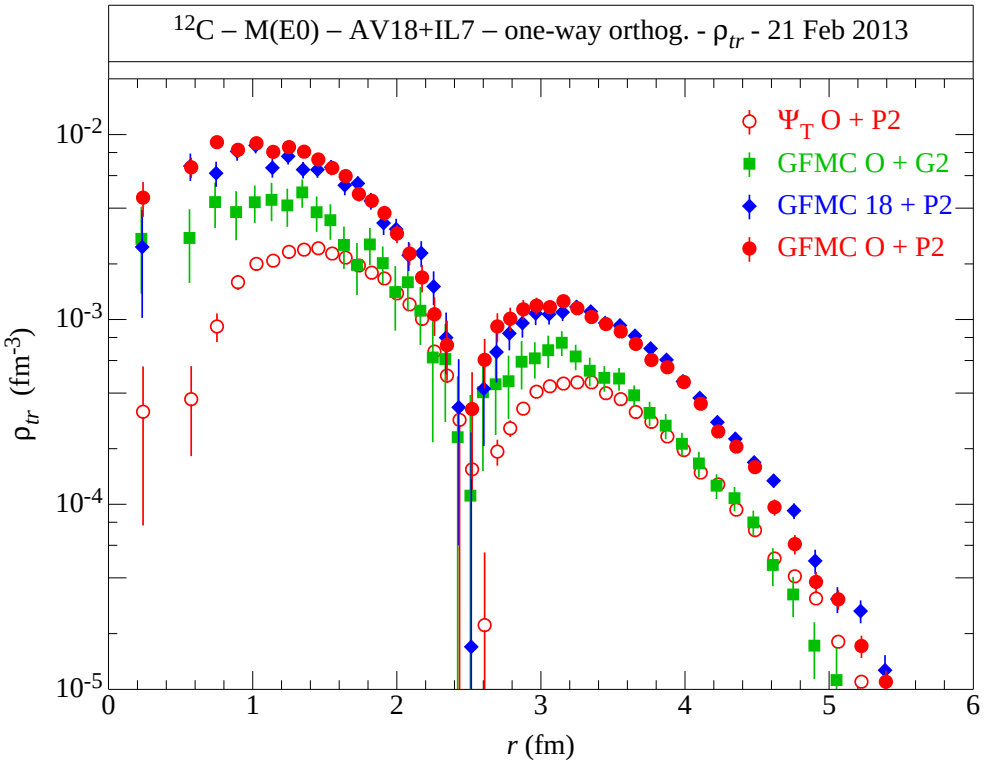
Define $\rho_{tr}(r) = \sum_i h0_2^+ j\delta(r \quad r_i)P_p j$g.s.$i$; $f_{tr}(k)$ is Fourier transform

$M(E0)$ $\int dr r^2 r^2 \rho_{tr}(r)$

Difficult to obtain exact orthogonality of (g.s.) and (0_2^+) in QMC;
we orthogonalize (0_2^+) to (g.s.) in the same walks used for $f_{tr}(r)$

$^{12}\mathrm{C}(\mathrm{g.s.})$! $^{12}\mathrm{C}(0_2^+)$ $\rho_{tr}(r)$



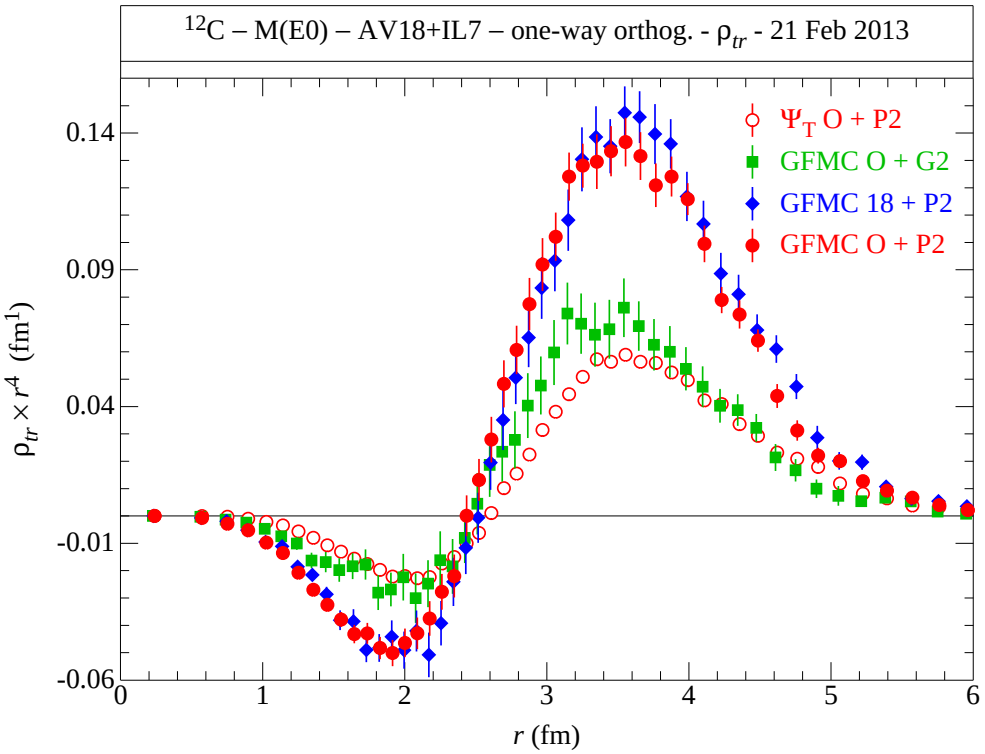


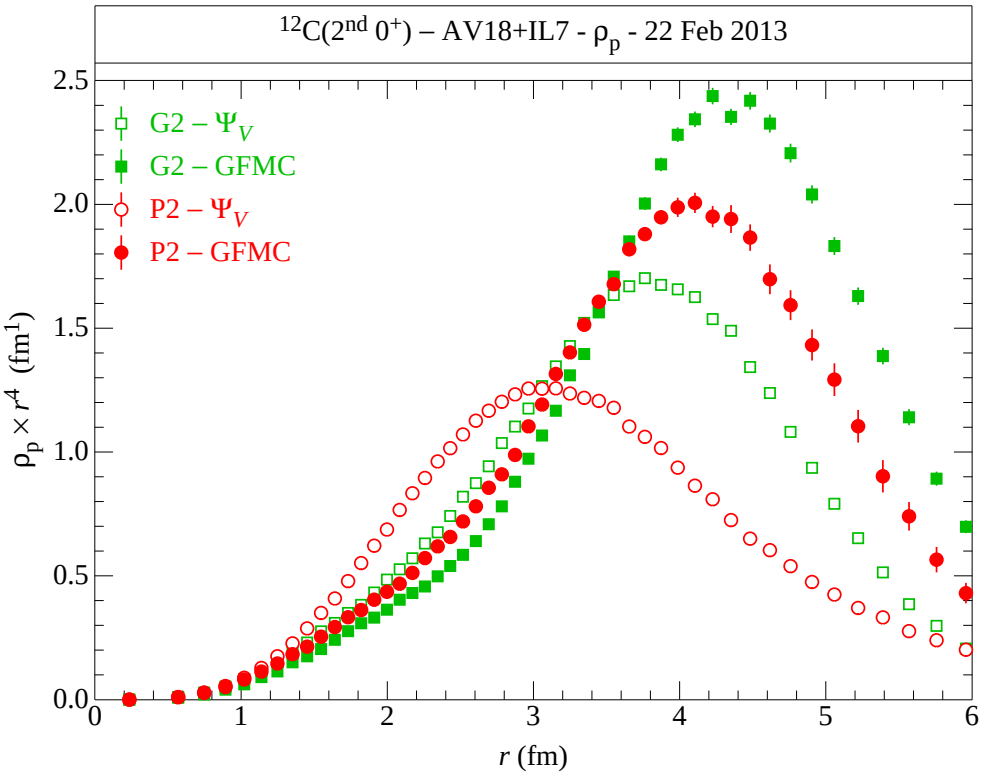
GFMC makes large correction to VMC ($_T$) result

Results are the same for two different g.s. calculations (O & 18)

Older 0_2^+ calculation gives much smaller $\rho_{tr}(r)$

$^{12}\mathrm{C}(\mathrm{G.S.})\ !\ ^{12}\mathrm{C}(0_2^+)\ \rho_{tr}(r)\quad r^4$





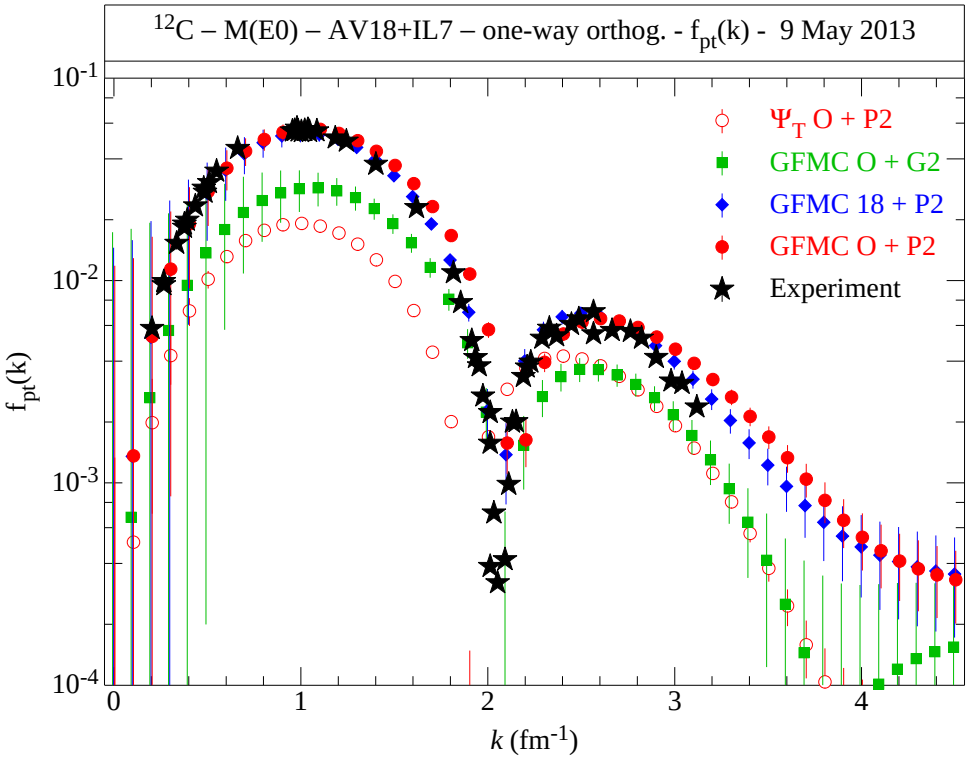
r^4 weighting corresponding to $M(E0)$

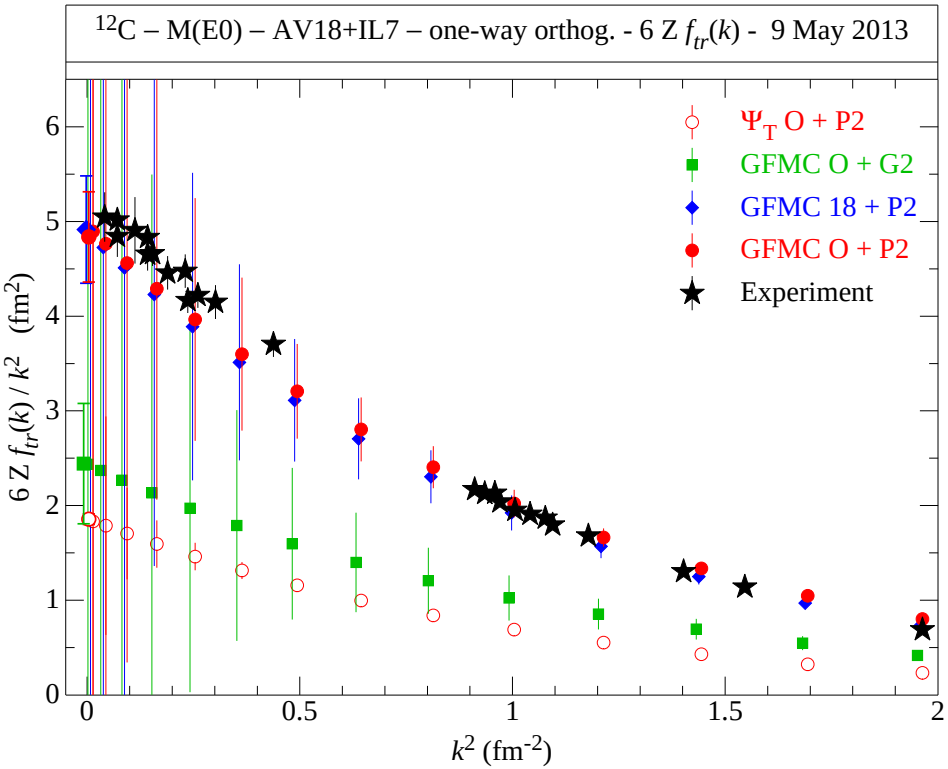
$\rho_{tr}(r)$ from two 0_2^+ calculation differ at all r

0_2^+ densities very different only for $r > 4$ fm

Different $\rho_{tr}(r)$ results due to many-body overlaps

^{12}C(G.S.) ! ^{12}C(0_2^+) f_{tr} FORM FACTOR





Data from M. Chernykh *et al.*, Phys. Rev. Lett. **105**, 022501 (2010)

Right panel $[f_{tr}(k)/k^2]$ proportional to $M(E0)$ at $k = 0$

Large errors at small k due to large Monte Carlo errors

Can get better value at $k = 0$ by computing $\int dr r^2 r^2 \rho_{tr}(r)$

Results with best 0_2^+ wave function in good agreement with data

^{10}C ! ^{10}B Fermi Beta Decay

One of the Fermi Beta decays being used to determine the v_{ud} CKM matrix element

Extracting v_{ud} requires a reliable value of the nuclear matrix element

If ^{10}C & ^{10}B wave functions are isospin symmetric, $\delta_c = 1$ $\frac{1}{2}jh^{10}\mathrm{B}\ j\ \mathrm{F}\ j\ ^{10}\mathrm{C}\ ij^2 = 0$

Up to now, GFMC calculations have assumed isospin conservation to save time

Can still have non-isospin symmetric ^{10}C & ^{10}B w.f., both with good T=1,
by propagating each with different Z

AV18 contains charge-independence breaking (CIB) terms: strong & E.M.

These could be important for determining the small departure of δ_c from 0.

Have enhanced GFMC to work in pn total charge basis
– GFMC wave function has components for all allowed total isospins
– A=10 w.f. have 2.5 more components

Wave function times on one Blue Gene/P node using 4 OMP cores

	^{10}C			^{10}B		
	Components	milli sec	MFLOPS	Components	milli sec	MFLOPS
Good isospin	46,080	218	1201	46,080	218	1201
Charge basis	107,520	164	1930	129,024	251	1636

Time does not scale with number of components

τ τ operation is much simpler for charge basis

CPU more efficient with longer inner loops (The more you spend, the more you save)

^{10}C & ^{10}B WITH CHARGE-INDEPENDENCE BREAKING

	^{10}C		^{10}B	
	Good T basis	pn basis	Good T basis	pn basis
Energies (MeV)				
Total	-59.99(19)	-60.15(16)	-62.91(16)	-62.77(13)
CIB	0.148(6)	0.045(4)	-0.118(9)	-0.219 8)
E & M	7.890(31)	7.877(24)	5.506(20)	5.452(18)
r_p r_n	0.28(1)	0.28(1)	0.	-0.03(1)
% T=0	-	–	-	0.077%
% T=2	-	0.010%	-	0.0053%
% T=3	-	0.0033%	-	0.0050%

Total energies not accurate enough to see improvement from charge basis

Can see clear improvement in NN CIB terms

Some signal of improvement in E&M terms

Non T=1 components are very small

CHARGE-INDEPENDENCE BREAKING IN NN SCATTERING

All calculations of ^{10}C ! ^{10}B have used only Coulomb CIB

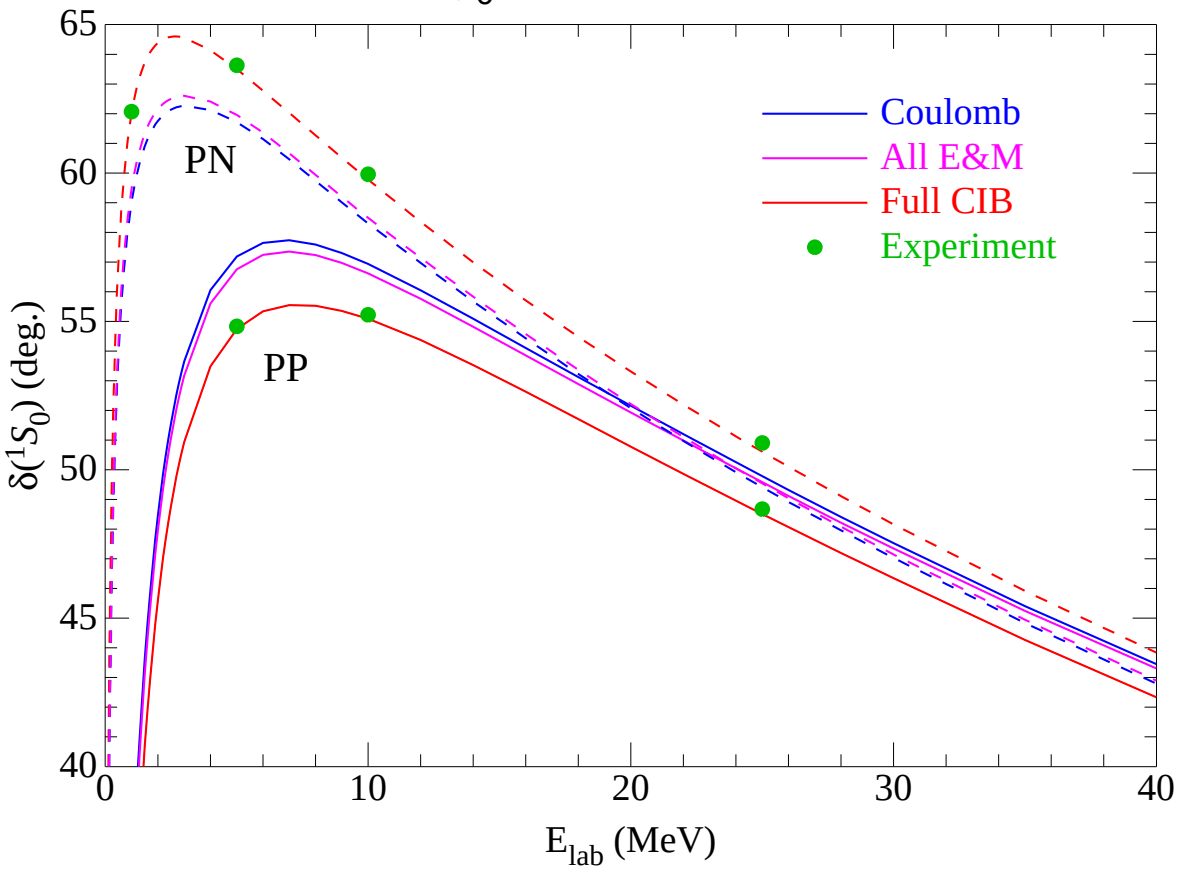
But there are other E&M terms: magnetic moment interactions, etc

And strong CIB interactions – isovector and isotensor (v_{15}–v_{18} in AV18)

Scattering lengths (fm)

CIB terms	$^1a_{pp}$	$^1a_{pn}$	$^1a_{nn}$
Coulomb	–8.46	–20.33	–20.33
All E&M	–8.35	–20.82	–19.94
Full CIB	–7.82	–23.73	–18.49
Experiment	–7.81	–23.75	–18.5(4)

$^1S_0$ Phase shifts



^{10}C ! ^{10}B Fermi Beta Decay

CIB terms	δ_C VMC	δ_C GFMC
AV18 + IL7; Cluster $_T$:		
Coulomb	.00122(5)	.00157(43)
All E&M	.00133(5)	.00216(24)
Coulomb + Strong	.00142(6)	.00273(23)
Full CIB	.00274(4)	.00412(24)
AV18 + IL7; S.M. $_T$:		
Full CIB	.00168(4)	.00329(16)
AV8', no V_{ijk}; S.M. $_T$:		
Full CIB	.00172(6)	.00282(23)
Following have only Coulomb		
Towner & Hardy a)	.0017	
W. Satula, *et al.* b)	.0065(14)	
"Expt." b)	.0037(15)	

a) Phys. Rev. C. **77**, 025501 (2008); b) Phys. Rev. C 86, 054316 (2012)

Full E&M terms (model independent) increase Coulomb-only δ_C by 40%

Full E&M + strong CIB terms more than double δ_C

CONCLUSIONS & FUTURE

Quantum Monte Carlo calculations of ^{12}C are making much progress

- ADLB library with OpenMP allows efficient use of $>$ 100,000 processors for GFMC
- Ground state of ^{12}C is well reproduced
- Hoyle state is not bad; E0 matrix element looks good
- First 2^+ energy also looks good

and there is still much to do

- 2^+ $E2$ form factor
- other ^{12}C states

Need to consider strong CIB interactions for ^{10}C beta decay

To Learn More

Pointers to the following are at http://www.phy.anl.gov/theory/staff/SCP.html & RBW.html

Nucleon-nucleon interactions, R. B. Wiringa, in Contemporary Nuclear Shell Models, ed. X.-W. Pan, D. H. Feng, and M. Vallières (Springer-Verlag, Berlin, 1997)

Monte Carlo calculations of nuclei, S. C. Pieper, in Microscopic Quantum Many-Body Theories and Their Applications, ed. J. Navarro and A. Polls, Lecture Notes in Physics **510** (Springer-Verlag, Berlin, 1998)

Quantum Monte Carlo Calculations of Light Nuclei, S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. **51**, 53-90 (2001)

Quantum Monte Carlo Calculations of Light Nuclei, S. C. Pieper, in Proceedings of the "Enrico Fermi" Summer School, Course CLXIX, ed. A. Covello, F. Iachello, and R. A. Ricci (Societ Italiana di Fisica, Bologna, 2008); arXiv:0711.1500 [nucl-th]

A simplified VMC program and description: *Variational Monte-Carlo Techniques in Nuclear Physics*, J. A. Carlson and R. B. Wiringa, Computational Nuclear Physics 1, ed. K. Langanke, J. A. Maruhn, and S. E. Koonin (Springer-Verlag, Berlin, 1990), Ch. 9 source & input files available at http://www.phy.anl.gov/theory/research/vmc-demo

ADLB load-balancing library is at http://www.cs.mtsu.edu/ rbutler/adlb

BIBLIOGRAPHY, CONTINUED

Detailed descriptions of the potentials

Accurate nucleon-nucleon potential with charge-independence breaking, R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38-51 (1995)

Realistic models of pion-exchange three-nucleon interactions Steven C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, Phys. Rev. C **64**, 014001-1:21 (2001)

Detailed descriptions of VMC and GFMC methods and many results

Quantum Monte Carlo calculations of nuclei with A 7, B. S. Pudliner, V. R. Pandharipande, J. Carlson, S. C. Pieper, and R. B. Wiringa, Phys. Rev. C **56**, 1720-1750 (1997)

Quantum Monte Carlo calculations of A=8 nuclei, R. B. Wiringa, Steven C. Pieper, J. Carlson, and V. R. Pandharipande, Phys. Rev. C **62**, 014001-1:23 (2000).

Quantum Monte Carlo calculations of A=9,10 nuclei, Steven C. Pieper, K. Varga, and R. B. Wiringa, Phys. Rev. C **66**, 044310-1:14 (2002).

Quantum Monte Carlo Calculations of Neutron-alpha Scattering, K.M. Nollett, S.C. Pieper, R.B. Wiringa, J. Carlson, G. M. Hale, Phys. Rev. Lett. **99**, 022502 (2007)

MICROSCOPIC FEW- & MANY-NUCLEON CALCULATIONS

Goal: a microscopic description of nuclear structure and reactions from bare NN & $3N$ forces.

There are two problems that must be solved to obtain this goal

(I) What is the Hamiltonian (i.e. the nuclear forces)?

NN force controlled by NN scattering – lots of data available

- Argonne v_{ij}

$3N$ force determined from properties of light nuclei

- Recent Illinois models with 2π & 3π rings

(II) Given H, solve the Schrödinger equation for A nucleons accurately.

Essential for comparisons of models to data

Quantum Monte Carlo has made much progress for A 12

Nuclei go up to A=238 and beyond!
– less accurate approximations are used beyond 12

Without (II) comparison to experiment says nothing about (I).

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

v_{ij}: Argonne v18 (1995)

$$v_{ij} = v_{ij}^{\gamma} + v_{ij}^{\pi} + v_{ij}^{R} + v_{ij}^{CIB}$$

v_{ij}^{γ}: pp, pn & nn electromagnetic terms, Coulomb, magnetic, etc. with form factors

v_{ij}^{π} $[Y(r_{ij})\sigma_i \ \ \sigma_j + T(r_{ij})S_{ij}] \ \ \tau_i \ \ \tau_j$; $\langle v_{ij}^{\pi} \rangle$ contributes 85% of $\langle v_{ij} \rangle$

$v_{ij}^{R} = \sum_{p=1,14} v_p(r_{ij}) O_{ij}^{p}$

$O_{ij}^{p=1,14} = [1, \sigma_i \ \ \sigma_j, S_{ij}, \mathbf{L} \ \ \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2\sigma_i \ \ \sigma_j, (\mathbf{L} \ \ \mathbf{S})^2] \ \ [1, \tau_i \ \ \tau_j]$

Determined phenomenologically

v_{ij}^{CIB}: 4 operators for nuclear charge independence breaking

AV18 is a direct fit to the Nijmegen data base:

1787 pp, 2514 pn, 1 nn data for $E_{Lab} < 350$ MeV 40 parameters; χ^2/d.o.f. = 1.09

Typical of 1990's NN potentials

R.B. Wiringa, V.G.J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, (1995)

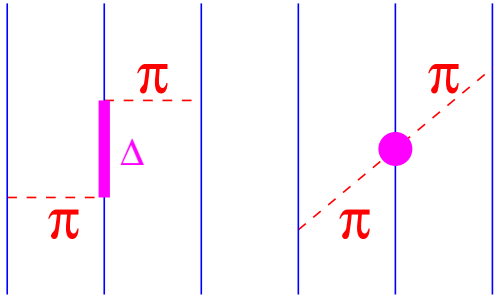
Nuclear Hamiltonian – Illinois V_{ijk}

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

$V_{ijk}^{2\pi}$: Fujita-Miyazawa + s-wave term; in most V_{ijk}

Longest ranged V_{ijk}

Attractive in all nuclei studied.



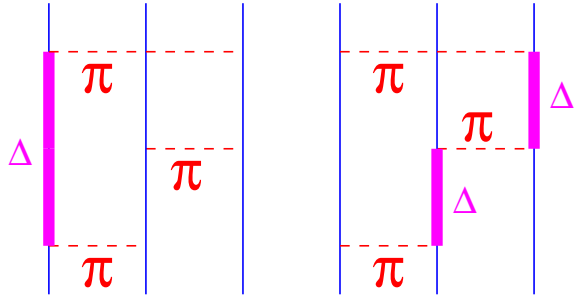
$V_{ijk}^{3\pi}$: 3π rings with 's; new in Illinois V_{ijk}

Extra p-shell, jN Zj attraction

One in energy denominator

2 , 3 denominators not yet considered

$\langle V_{ijk}^{3\pi} \rangle < 0.1 \langle V_{ijk}^{2\pi} \rangle$



V_{ijk}^{R}: represents all else including relativistic effects – purely central and repulsive

3-4 Couplings adjusted to fit 17 nuclear levels for A 8

In light nuclei we find $\langle V_{ijk} \rangle$ (0.02 to 0.09)$\langle v_{ij} \rangle$ (0.15 to 0.6)$\langle H \rangle$

(Large cancellation of K and v_{ij})

We expect $\langle V_{4N} \rangle$ 0.06$\langle V_{ijk} \rangle$ (0.02 to 0.04)$\langle H \rangle$ (0.5 to 2.) MeV

But not possible to disentangle from V_{ijk} uncertainties.

S.C. Pieper, V.R. Pandharipande, R.B. Wiringa, and J. Carlson, Phys. Rev. C **64**, 014001 (2001)

Pieper, AIP CP **1011**, 143 (2008)

THE MANY-BODY PROBLEM

Need to solve

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

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

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

$2^A \quad \binom{A}{Z}$ complex coupled 2^{nd} order eqn in $3A$ variables

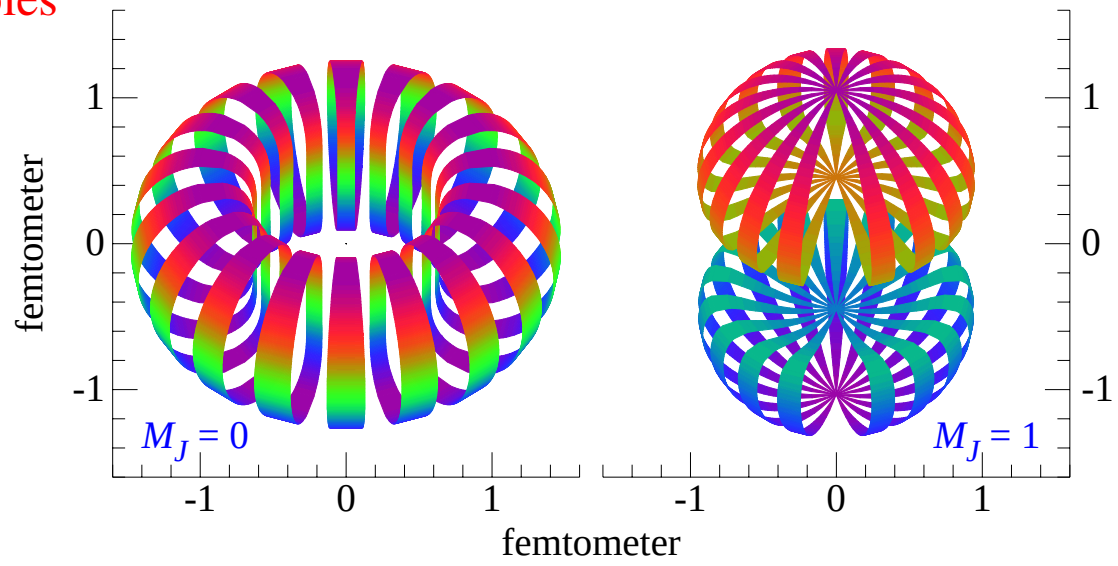
(number of isospin states can be reduced)

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

Coupling is strong:

$\langle v_{\text{Tensor}} \rangle$ is 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

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \qquad E_0$$

Monte Carlo integration (Metropolis random walk) is used for the $3A$-dimensional integral

Simplified trial wave function:

$$|\Psi_T\rangle = \mathcal{S} \prod_{i<j} \left[1 + U_{ij} + \sum_k U_{ijk} \right] \prod_{i<j} f_{ij} |\Phi\rangle$$

is a fully antisymmetric combination of one-body wave functions $\phi_i(\vec{r_j})$

determines quantum numbers of state

translationally invariant – written in terms of $\vec{r_i} \qquad \vec{R_{\rm cm}}$

has multiple spatial-symmetry components; usually in LS basis

Can be made with arbitrary $\phi_i(\vec{r_j})$,

e.g. solutions, with correct asymptotic behavior, of Woods Saxon potentials

Can have sub-cluster structure, like α+t+n for ^{8}Li or α+α+α for ^{12}C

f_{ij} are central (mostly short-ranged repulsion) correlations

U_{ij} are non-commuting 2-body correlations from v_{ij}

U_{ijk} are 3-body correlations from V_{ijk}

GREEN'S FUNCTION (DIFFUSION) MONTE CARLO

VMC $_T$ propagated to imaginary time τ:

$$(\tau) = e^{(H \quad E_0)\tau} \quad _T$$

$$_T = \quad _0 + \sum \alpha_i \quad _i \quad ; \qquad (\tau) = e^{(E_0 \quad E_0)\tau} \quad [\quad _0 + \sum \alpha_i e^{(E_i \quad E_0)\tau} \quad _i]$$

$$_0 = \lim_{\tau \,!\, 1} \quad (\tau) \quad ; \quad H \quad _0 = E_0 \quad _0$$

Small imaginary-time-step propagator:

$$(\tau) = \left[e^{(H \quad E_0)\,4\,\tau}\right]^n \quad _T; \quad \tau = n\,4\,\tau$$

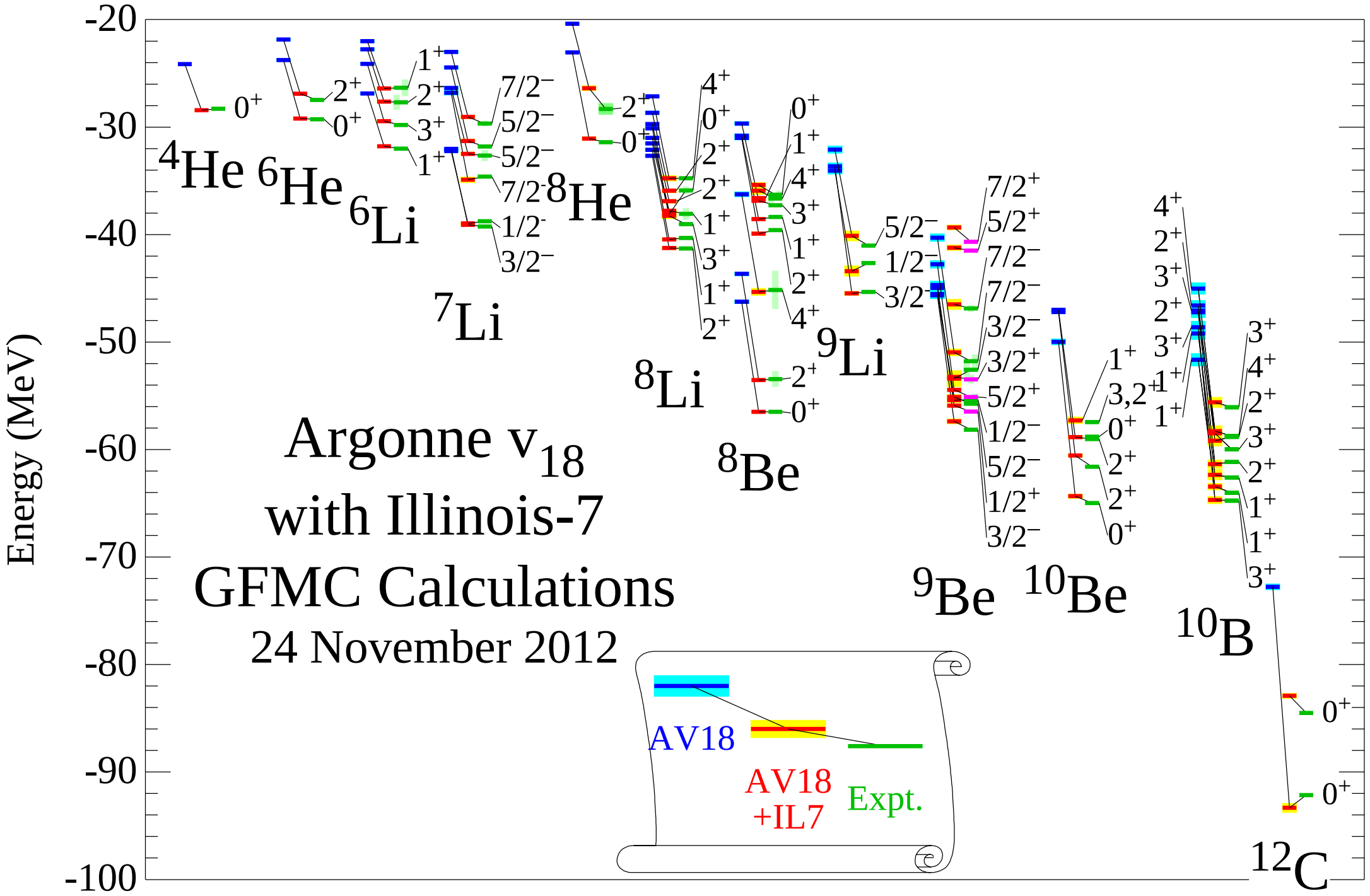
Can be computed to order $(4\tau)^3$

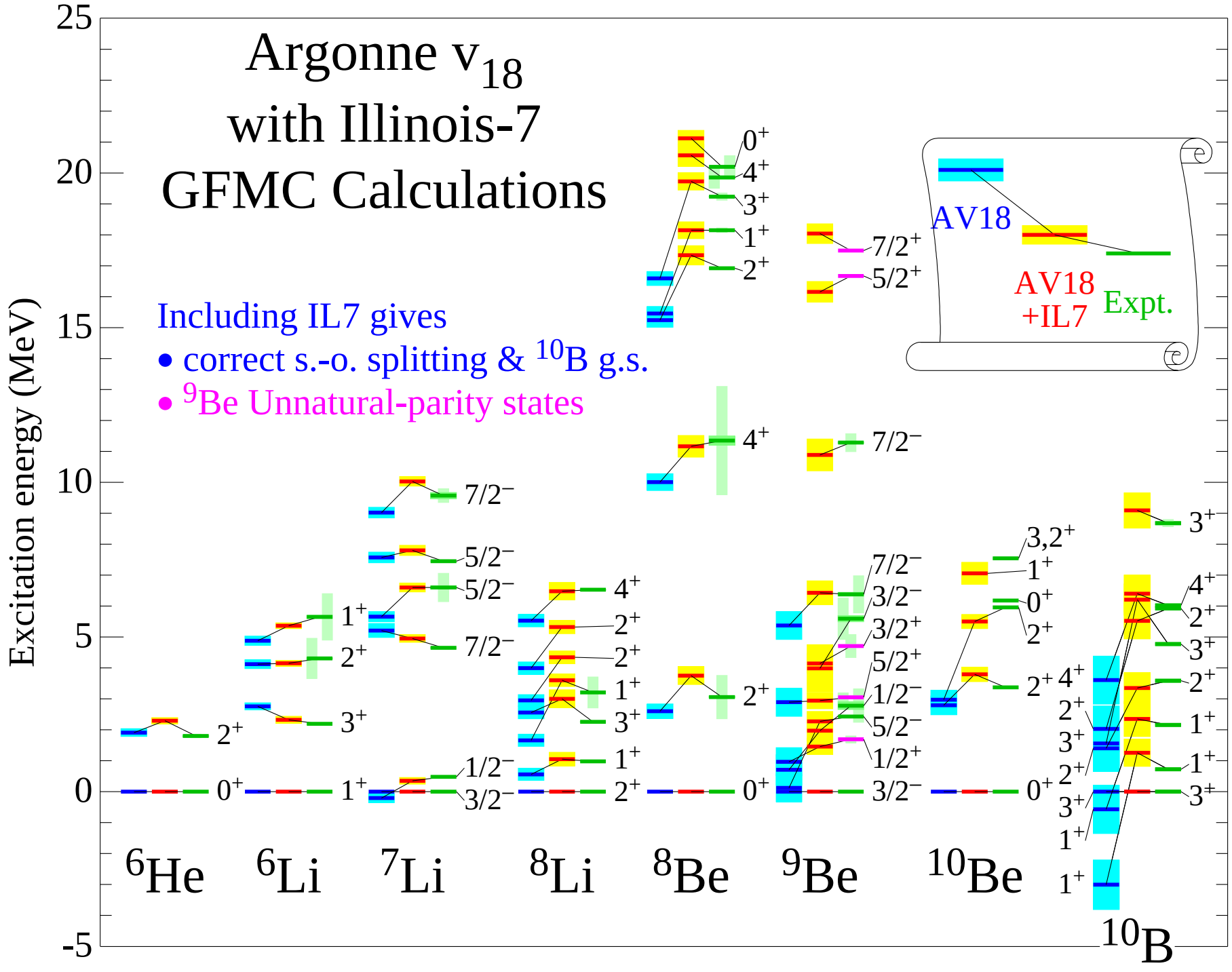
$$G_{\beta\alpha}(\mathbf{R}^0, \mathbf{R}) = h\mathbf{R}^0, \beta j e^{(H \quad E_0)\,4\,\tau} j\mathbf{R}, \alpha i$$

$$(\mathbf{R}_n, \tau) = \int G(\mathbf{R}_n, \mathbf{R}_{n \quad 1}) \quad G(\mathbf{R}_1, \mathbf{R}_0) \quad _T(\mathbf{R}_0) d\mathbf{R}_{n \quad 1} \quad d\mathbf{R}_0$$

$$E(\tau) = \frac{h \quad _T j H j \quad (\tau) i}{h \quad _T j \quad (\tau) i} \quad E_0$$

Done by Monte Carlo integration – $3An$ dimensions (typically 36,000 for ^{12}C)

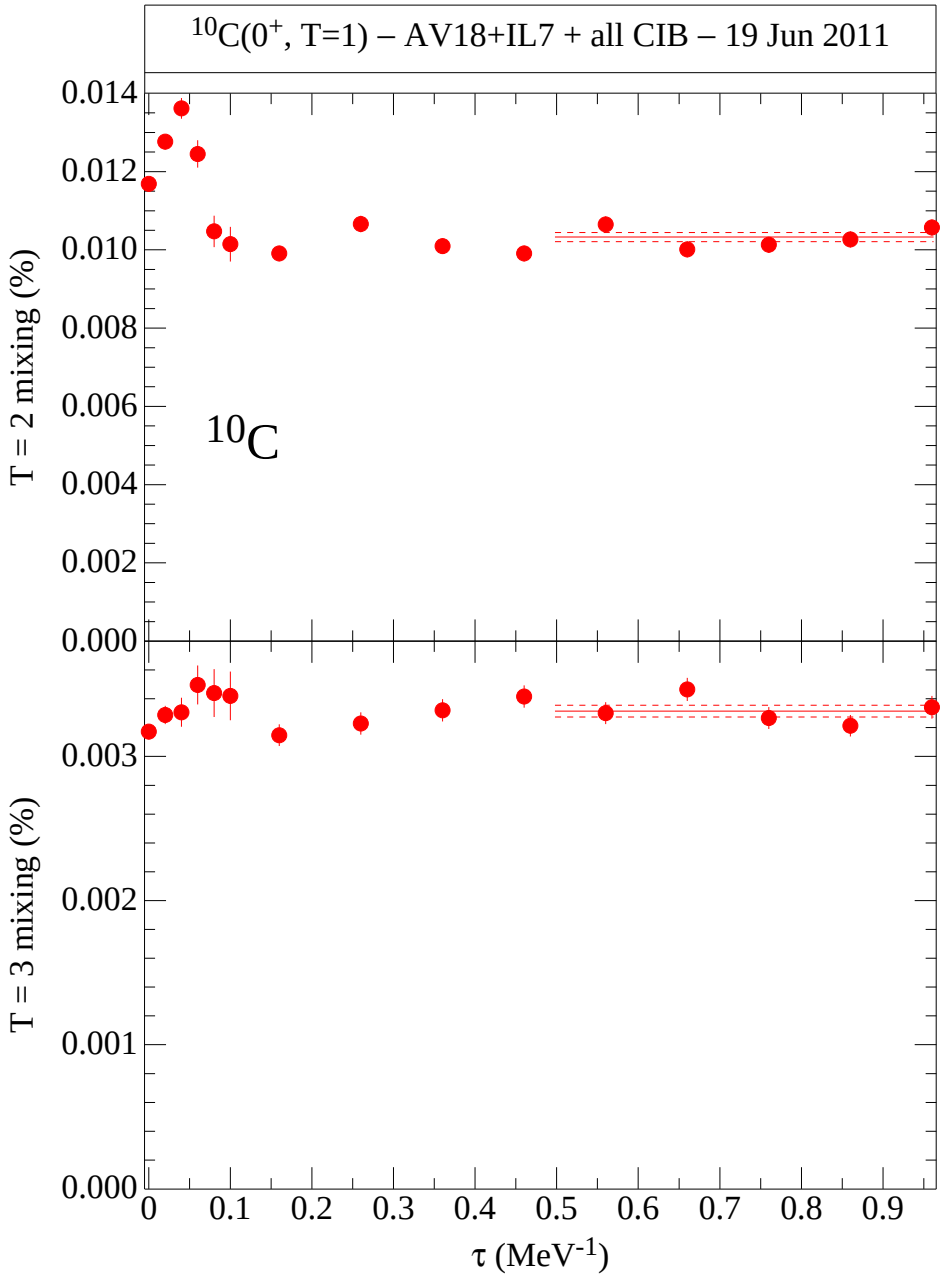

Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Be
10B
12C
Argonne v18
with Illinois-7
GFMC Calculations
24 November 2012
AV18
AV18
+IL7
Expt.

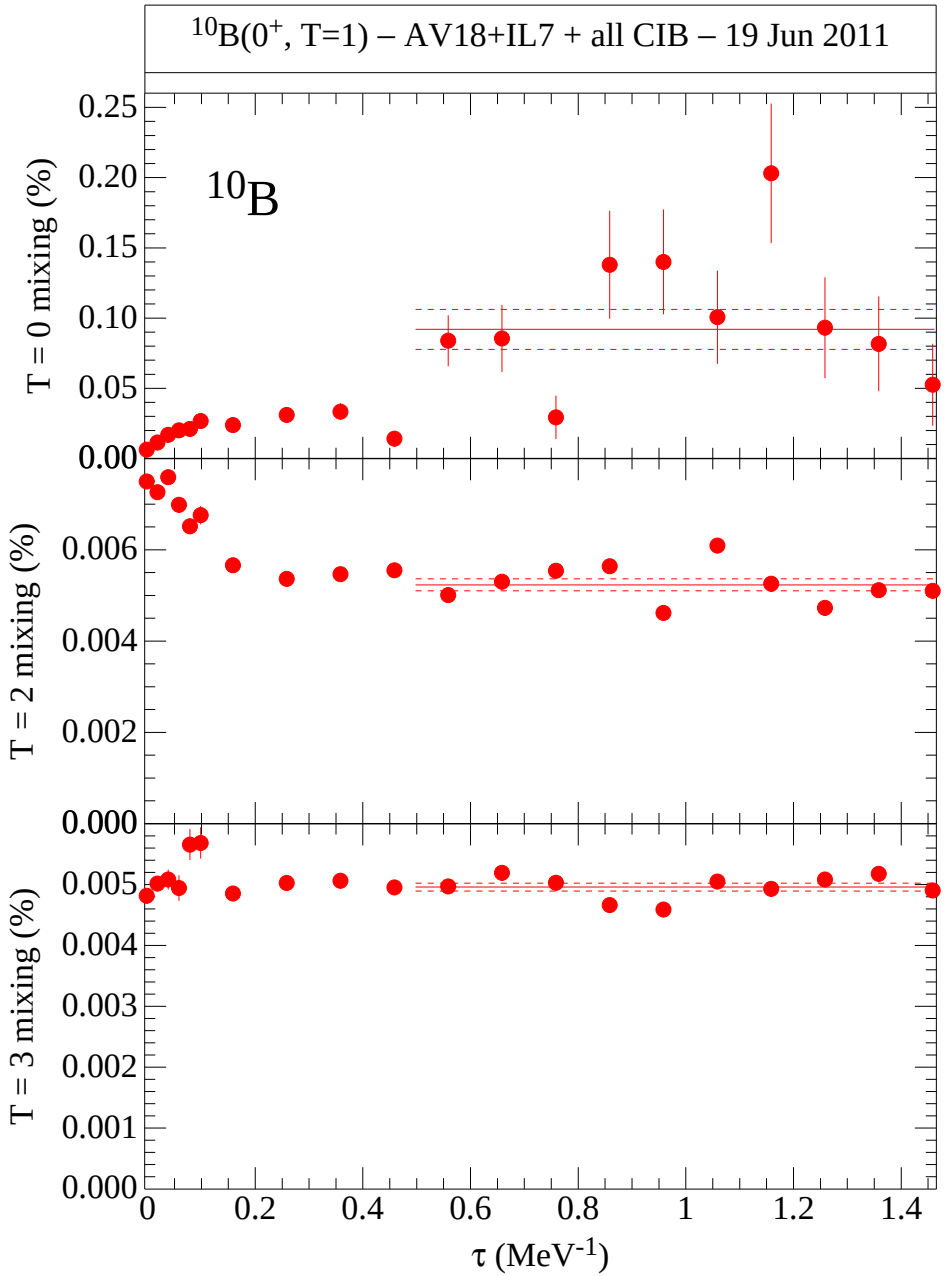

Argonne v18
with Illinois-7
GFMC Calculations
Including IL7 gives
• correct s.-o. splitting & 10B g.s.
• 9Be Unnatural-parity states
AV18
AV18
+IL7
Expt.
Excitation energy (MeV)
25
20
15
10
5
0
-5
6He
6Li
7Li
8Li
8Be
9Be
10Be
10B

Scaling of Ψ_T Calculation Time With Nucleus

	Pairs	Spin	Isospin	$\prod(/^8\mathrm{Be})$
^{4}He	6	8	2	0.002
^{6}Li	15	32	5	0.048
^{7}Li	21	128	14	0.75
^{8}Be	28	128	14	1.
^{8}Li	28	128	28	2.
^{9}Be	36	512	42	15.
^{10}B	45	512	42	19.
^{10}Be	45	512	90	41.
^{11}Li	55	2048	110	247.
^{12}C	66	2048	132	356. ! 500.
^{16}O	120	32768	1430	112,065.
^{40}Ca	780	$3.6\ 10^{21}$	$6.6\ 10^{9}$	$5.6\ 10^{19}$

^{10}C & ^{10}B WITH CIB – PRELIMINARY





What is happening with ^{10}B T=0?

FERMION-SIGN PROBLEM & CONSTRAINED-PATH PROPAGATION

The Fermion sign problem limits maximum τ:

G brings in lower-energy boson solution

$h \quad _T j H j \quad (\tau) i$ projects back antisymmetric solution

Exponentially growing statistical errors

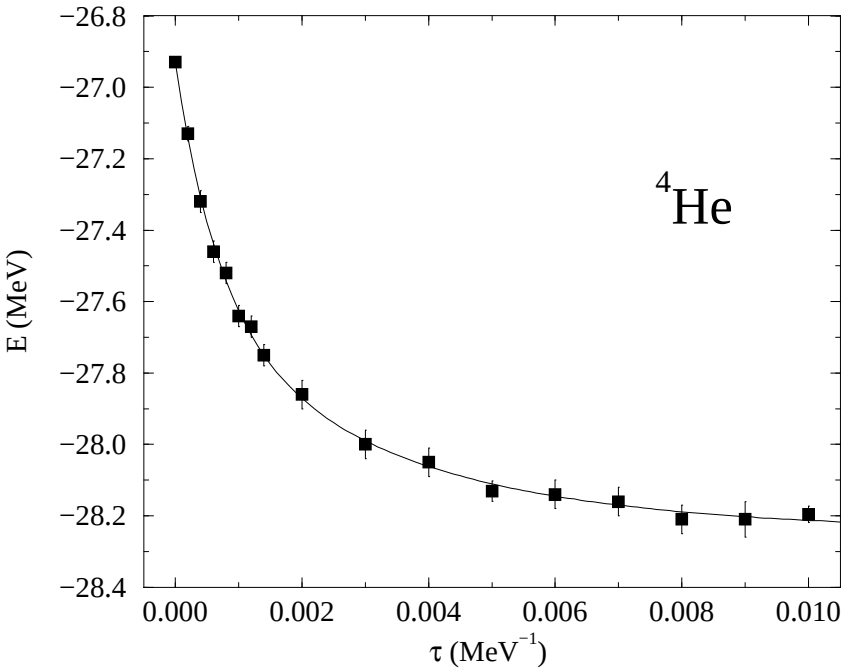
Constrained-path propagation (Joe Carlson), removes steps that have

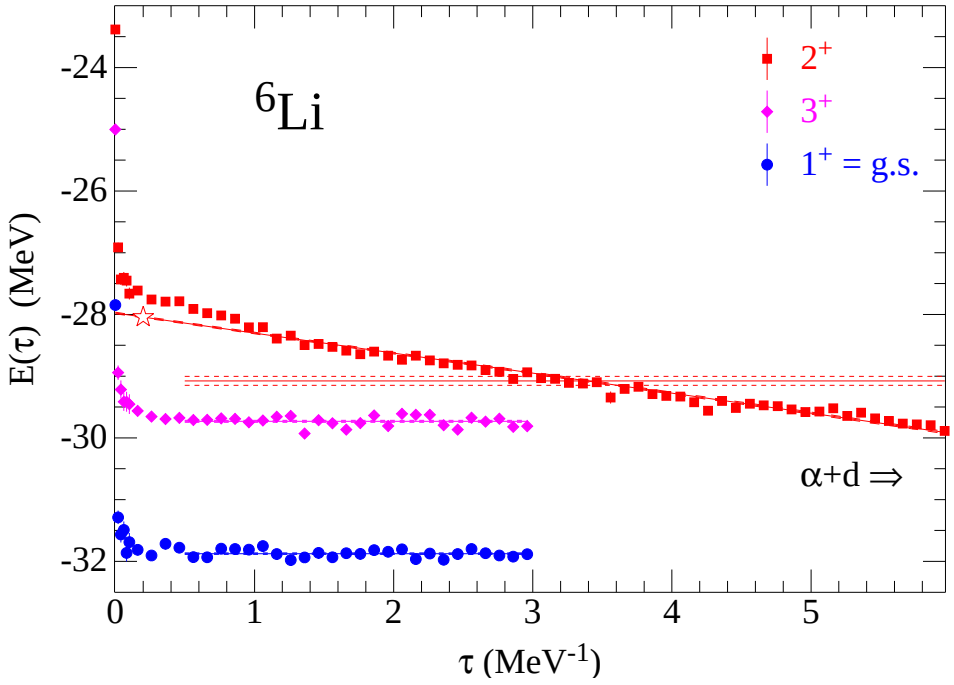
$$\overline{\quad\quad\quad\quad\quad\quad} \quad {}^{y}_{T}(\mathbf{R}) \quad (\tau, \mathbf{R}) = 0$$

Any resulting errors (bias) are removed by 20 40 unconstrained steps before evaluating observables.

Have to check for each significantly different problem

Examples of GFMC Propagation





Curve has $\sum \exp(E_i \tau)$ with
E_i = 20.2, 340 & 1480 MeV
(20.2 MeV is first ^{4}He 0^+ excitation)
τ 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 estimate of resonance energy
Should use scattering boundary conditions
Have done n+^{4}He, doing n+^{3}H & p+^{3}He

MAKING GFMC WORK ON 131,072 PROCESSORS OF BG/P

GFMC needed to be redone for leadership class computers

- Old program did several Monte Carlo samples per processor
- Branching can kill samples – need enough not to fluctuate to zero
- ^{12}C has only 15,000 Monte Carlo samples
- Leadership class computers have many 10,000's processors
- Need to split one sample over many processors

Argonne's IBM Blue Gene/P

Automatic Dynamic Load Balancing (ADLB) for sharing work between nodes

- A general-purpose library to help application codes dynamically share work
- Developed by Rusty Lusk and Ralph Butler under UNEDF SciDAC
- GFMC was principal needs driver and test bed
- Good efficiency on 32,768 nodes (4 rows, 32 racks, 131,072 processors) of BG/P

OpenMP allows the 4 cores on one node to work together on one piece of work

- Full memory of node is used for just 1, not 4, tasks
- Efficiency is very good – 4 cores are 3.8 faster than 1 core

ADLB is a general purpose library; give it a try! – http://www.cs.mtsu.edu/ rbutler/adlb

ADVANCING FROM THE IBM BG/P TO THE BG/Q

ADLB under UNEDF resulted in code working well on BG/P:

– 2 Gbytes and 4 cores (each one thread) per node

– ^{12}C(0^+) needs 2 Gbytes so OpenMP used for the 4 cores (threads)

– ADLB gives excellent scaling to 32,768 nodes

BG/Q offers new possibilities and challenges

– 16 Gbytes, 16 cores (each 4 threads) per node

– 48 1024 nodes

– ^{12}C(0^+): 8 ranks/node (8 threads each) or 4, 2, or 1 (64 threads)

– Other ^{12}C states need much more memory/rank (T=1: 14 Gbytes)

Early Science grant gave access to machine as it was still being installed

– One must be patient!

Conversion went very well

– ADLB performance even better on BG/Q with no modifications!

– OpenMP scales well to more threads

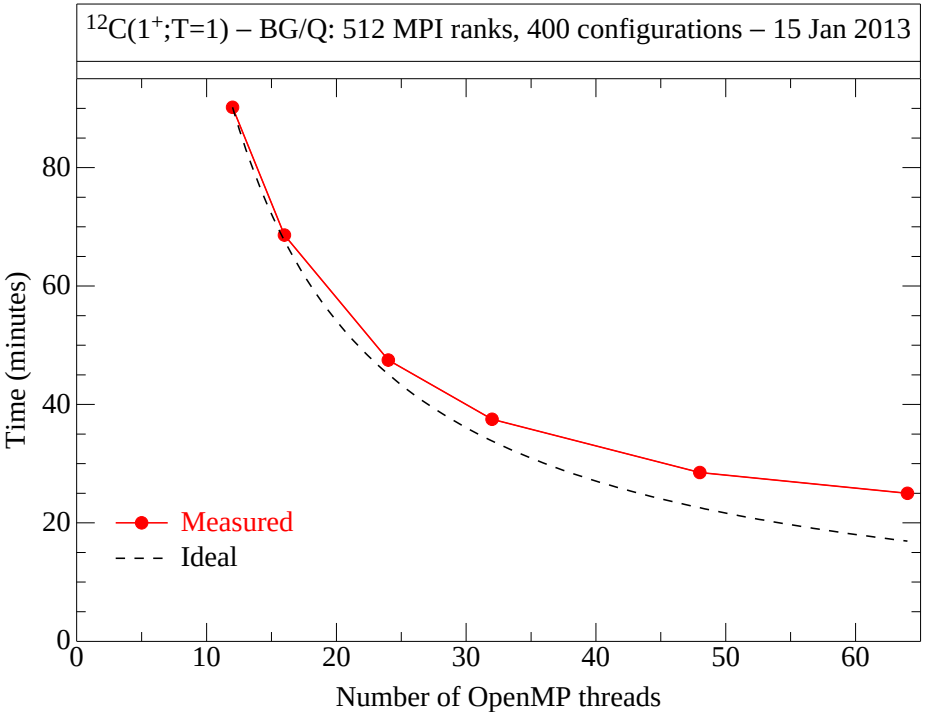
SCALING FOR $^{12}C(1^+;T=1)$

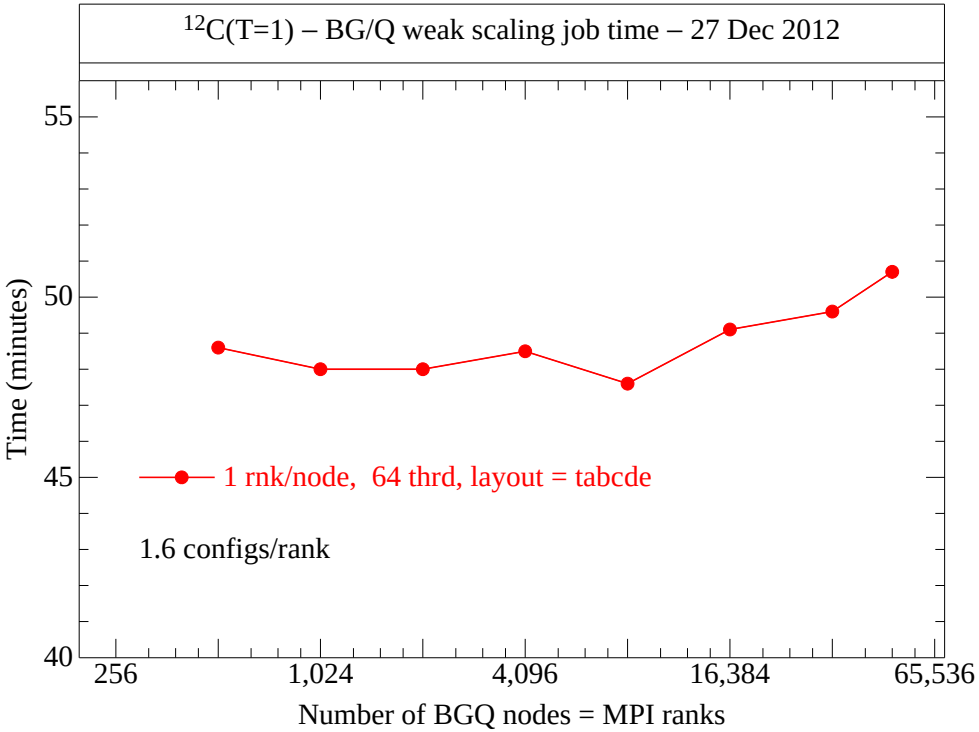
14 Gbytes per rank – only one rank/node possible

OpenMP keeps improving all the way to 64 threads

Good scaling to full machine (48 1024 nodes or ranks)

Impossible calculation on BG/P





First Physics Results on Mira (BG/Q)

Machine accepted and made available just before Christmas

Have made initial VMC $_T$ and GFMC propagations for

– $^{12}C(2^+)$, E = 3.9(1.0) vs Expt. = 4.44

– $^{12}C(1^+;1)$, E = 21.6(1.3) vs Expt. = 15.11

Not possible on BG/P because of large (up to 14 GBytes/rank) memory needs