Quantum Monte Carlo
as a tool for astrophysics

Ken Nollett
Argonne
21 August 2005
Frontiers 2005

Co-conspirators: Joe Carlson & Gerry Hale (Los Alamos)
Steve Pieper & Bob Wiringa (Argonne)
Rocco Schiavilla (Jefferson Lab / Old Dominion)

Office of Science
U.S. DEPARTMENT OF ENERGY

Office of Nuclear Physics
Exploring Nuclear Matter - Quarks to Stars

THE UNIVERSITY OF CHICAGO

ARGONNE NATIONAL LABORATORY

A lot of nuclear theory, especially as used in astrophysics, is top-down, in the sense that it is fitted to data for complex systems, and is in some sense curve-fitting

Something that will definitely not be curve-fitting, if it works, is describing nuclei and their reactions in terms of the vacuum nucleon-nucleon interaction

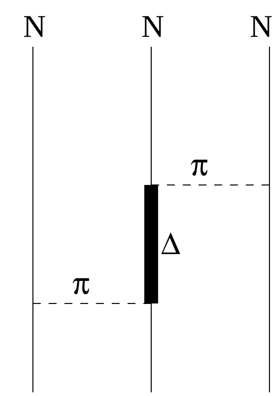
Success over a range of masses would tell us that nuclei are in fact made of protons and neutrons (not just effective in-medium p and n) and would let us predict with confidence quantities like low-energy cross sections that otherwise constitute expensive and heart-breaking experimental work

Seeing whether it can be done (and as a practical matter, it may only be possible in light systems) has motivated a lot of good work over the last dozen years, and it provides an opportunity for astrophysics

"Realistic" interactions fit the pp, np, and deuteron data with $\chi^2_\nu \lesssim 1.10$ and $\nu \simeq 4300$

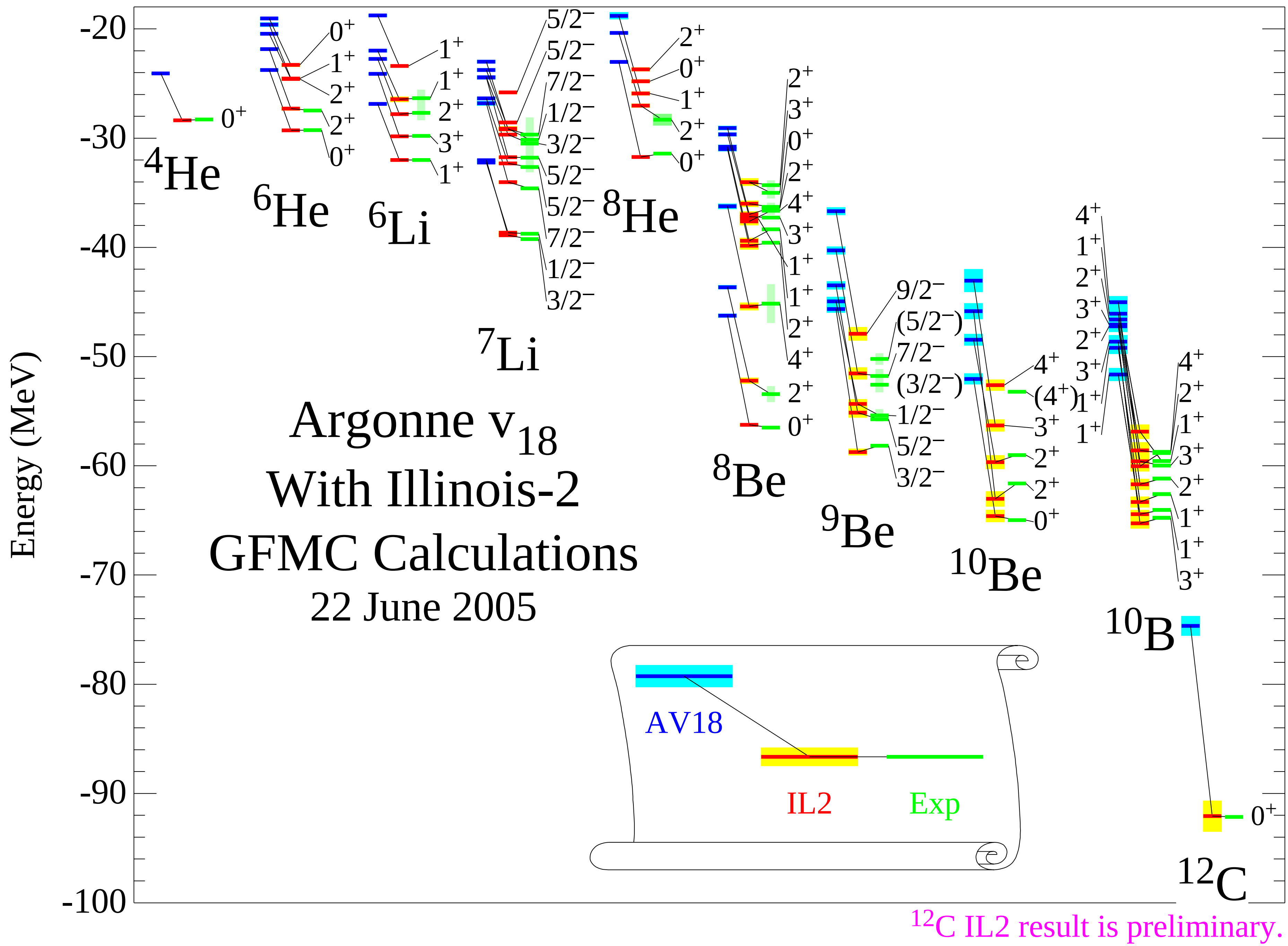
I work with the Argonne v_{18} potential (AV18), which contains 18 operator terms, plus EM & π-exchange terms – 40 parameters adjusted one time to the data 10 years ago

The 3-body interaction is important because our wave functions contain no explicit π or Δ degrees of freedom – have to have NNN interaction to get $A = 3$ and higher masses correct



The 4-body interaction is expected to be much less important – we fit our 3-body force to 17 states at $A \leq 8$ and see that it does quite well

Our current three-body interaction is Illinois 2 (IL2)


Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
4He
6He
6Li
7Li
8He
8Be
9Be
10Be
10B
12C
Argonne v18
With Illinois-2
GFMC Calculations
22 June 2005
AV18
IL2
Exp
12C IL2 result is preliminary.

The complicated potential requires good methods to compute nuclear properties

The Schrödinger equation is

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A)$$

where $\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_A)$ is a function of all particle separations and a vector in spin and isospin

This comes out to 270,336 coupled equations in 33 variables for ^{12}C

We use two methods of solution:

Variational Monte Carlo (VMC) is based on adjusting parameters in a complicated Ansatz for Ψ to minimize $\langle \hat{H} \rangle$ as found by Monte Carlo integration

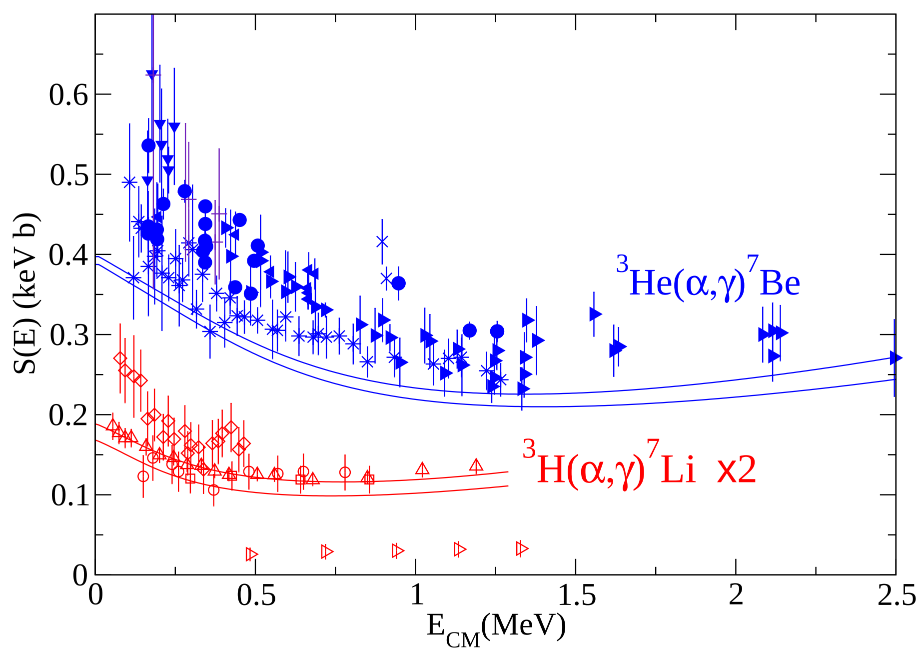
Green's Function Monte Carlo (GFMC) takes Ψ_T from VMC and finds the true ground state as

$$\Psi(\tau) = \exp\left[-(\hat{H} - E_0)\tau\right] \Psi_T$$

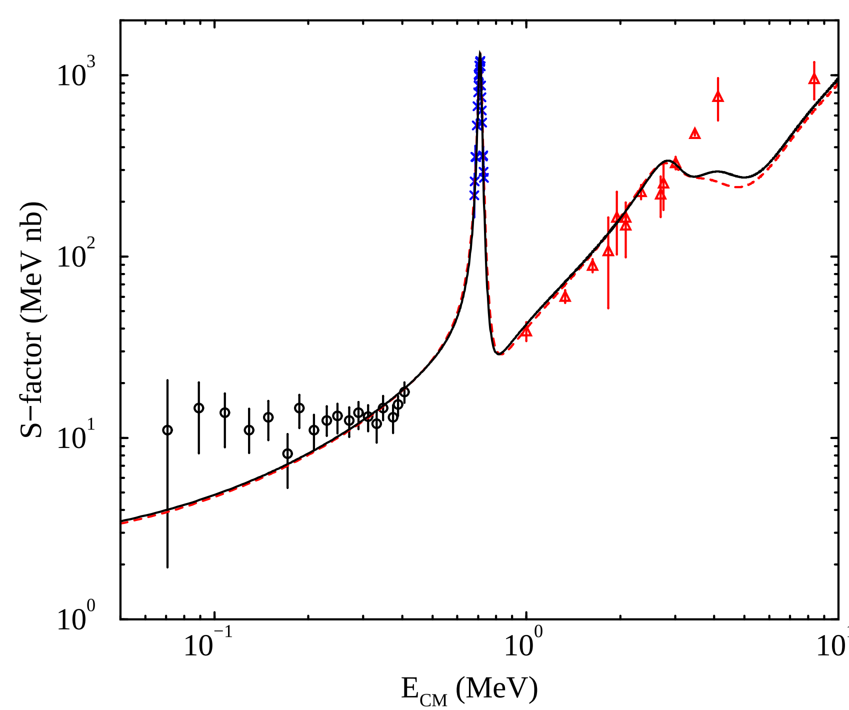
with $\tau \longrightarrow \infty$

We can take these methods and adapt them to scattering and reactions

As a first pass, we computed (α, γ) cross sections using VMC plus some phenomenological information



$^2H(\alpha, \gamma)^6Li$

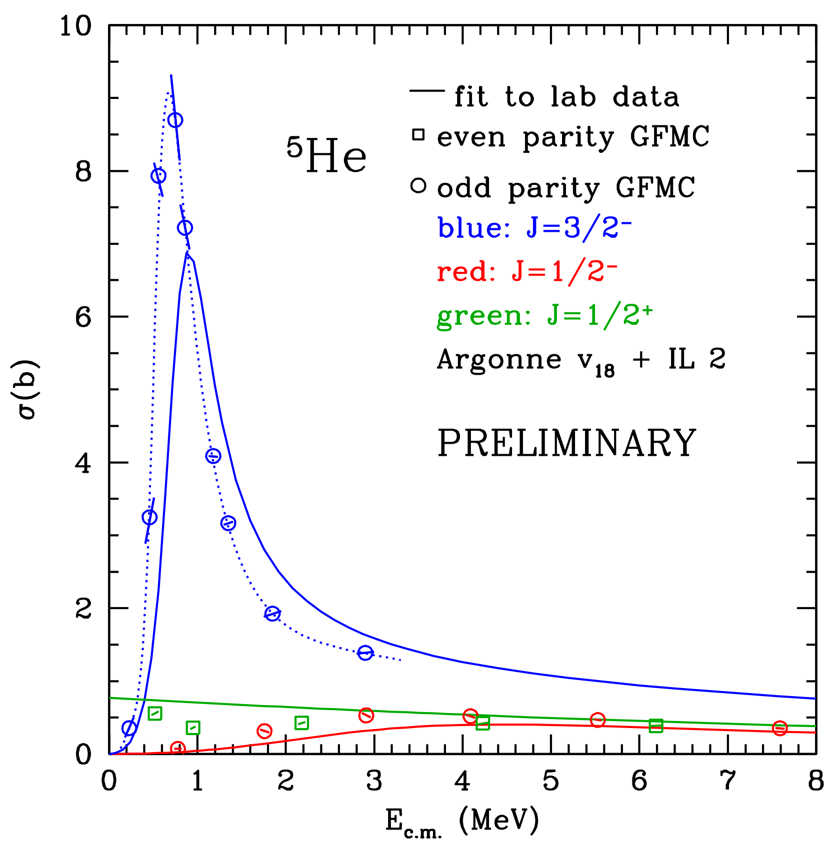


The result was encouraging, be we're not at a reliable, predictive theory yet

Two things are particularly needed:

1. Learning to compute continuum states from the NN+NNN potential
2. Machinery to use GFMC wave functions in matrix elements

We're at work on a simple but informative learning problem: ^{4}He + n

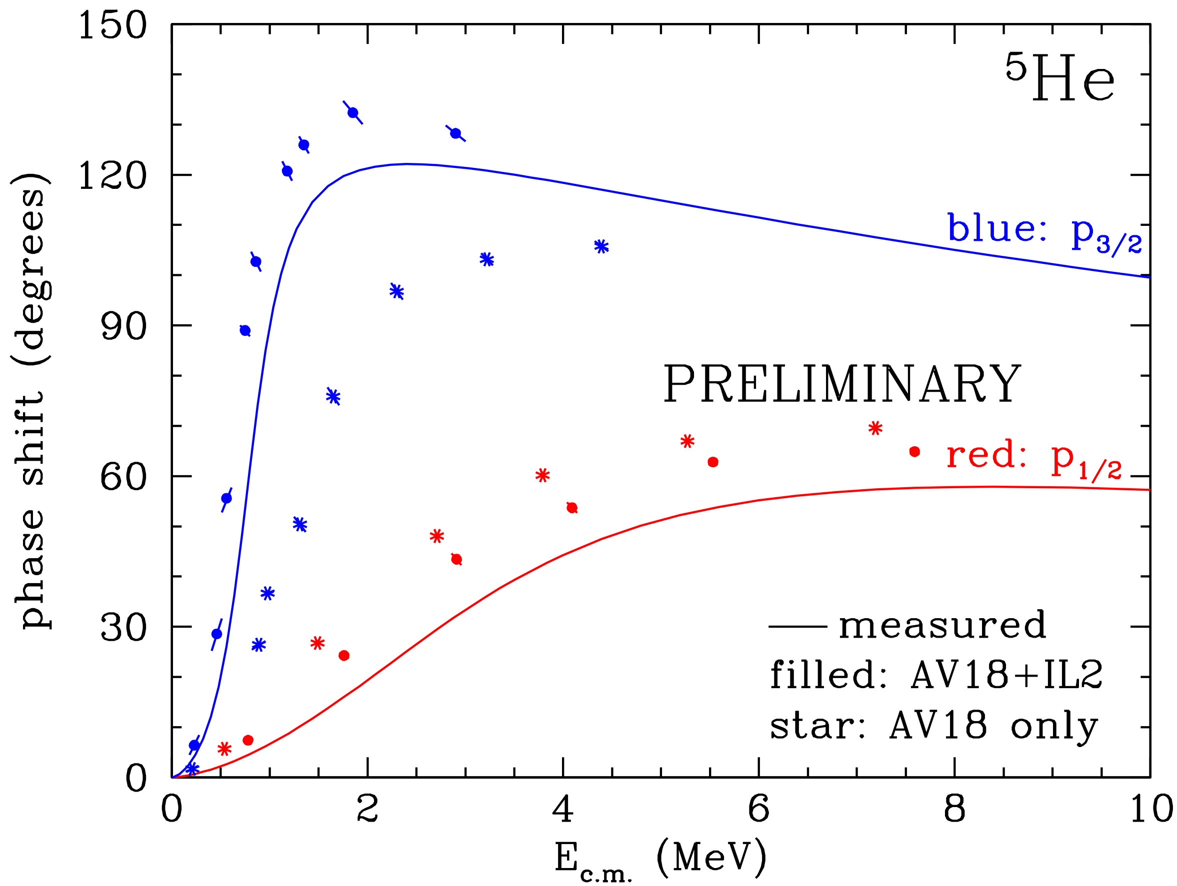


Confine system to spherical box with max αn separation R_0

Specify log derivative γ for the wave function at $r_{\alpha n} = R_0$

Methods give lowest-energy state for fixed γ

Calculations at varying γ map out $E(\gamma)$ and equivalently $\delta(E)$



With AV18+IL2, we reproduce the spin-orbit splitting very well

The overall scale is within 200 keV of experiment, compared with a 700 keV RMS deviation from experiment for 59 other p-shell states

What comes next

States in ^{4}H and ^{7}He

Lots of thermal-neutron scattering and capture at $A \lesssim 8$

$^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$	solar ν mixing
$^{7}\mathrm{Li}(n,\gamma)^{8}\mathrm{Li}$	r-process
$^{9}\mathrm{Be}(n,\gamma)^{10}\mathrm{Be}$	r-process
$\alpha\alpha n \longrightarrow {}^{9}\mathrm{Be} + \gamma$	r-process
$\alpha\alpha\alpha \longrightarrow {}^{12}\mathrm{C} + \gamma$	all burning & nucleosynthesis beyond He
$^{3}\mathrm{H}(\alpha,\gamma)^{7}\mathrm{Li}$	big bang, r-process
$^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$	solar ν mixing, big bang
	persistent systematic discrepancies in data
$d(\alpha,\gamma)^{6}\mathrm{Li}$	big bang
	E1 puzzle in reaction mechanism

Over the longer term, we should be able to address transfer reactions

The method as it stands will top out around $A = 12$, but more approximate versions may go to $A = 20$ or so, and there may be an opportunity to use QMC to calibrate less-microscopic methods