Quantum Monte Carlo:

Not Just for Energy Levels Anymore

Kenneth Nollett

3rd Argonne/MSU/INT/JINA RIA Theory Workshop

5 April 2006

work done by or with many collaborators:

J. Carlson • G. M. Hale

V. R. Pandharipande • S. C. Pieper

R. Schiavilla • K. Varga • R. B. Wiringa

with vital support from DOE Office of Science, NERSC, Argonne Laboratory Computing Resource Center, Argonne Math & Comp. Sci. Division, Los Alamos

Motivation

Given an interaction in vaccum, there are several computational approaches to nuclear systems, as you've been hearing:

No-core shell model with Lee-Suzuki or Bloch-Horowitz for Hamiltonian

Coupled clusters with G-matrix interaction

Density functional theory, granted an energy functional derived from the interaction

Quantum Monte Carlo – Variational Monte Carlo
Green's function Monte Carlo

The last two work directly with a bare interaction and bare operators and describe the wave function without expanding in basis functions, so they have rather different sets of advantages and disadvantages from the others

Advantages of gambling:

Avoid storage & processing demands of basis methods (at least if $A \leq 12$)

Not afflicted by fervent hope for a soft-core interaction or weak 3-body interaction

Intruder states are no more demanding than natural parity

No effective interactions, operators, or quenching to assume or construct

Extension to at least single-open-channel unbound states is straightforward

More advantages

Freedom from a basis also gets rid of a lot of basis-choice and convergence uncertainties

At a minimum, this lets us apply an interaction with different "systematic" issues than most other methods

This also makes QMC a good cross check for methods applicable at larger mass number

As with all methods, there are some disadvantages – in our case, the restriction to local interactions, the fermion sign problem, and difficulty producing the Green's function for some types of interaction terms

What we actually do, part I: Interactions

We work with the Argonne v_{18} nucleon-nucleon potential

It's one of several realistic potentials you've already heard about

- fits all pp & np data to 350 MeV in Nijmegen 1993 phase shift analysis with $\chi^2_\nu = 1.09$
- 18 operator terms ($\mathbf{L}\cdot\mathbf{S}, \sigma\cdot\sigma$, tensor, scalar...), $\sim$40 parameters fitted once ten years ago
- strong repulsive core, strong tensor interaction and π exchange at longer range
- full complication of EM interaction (mag. moment, vacuum polarization...), charge symmetry breaking, charge dependence

What we actually do, part I: Interactions

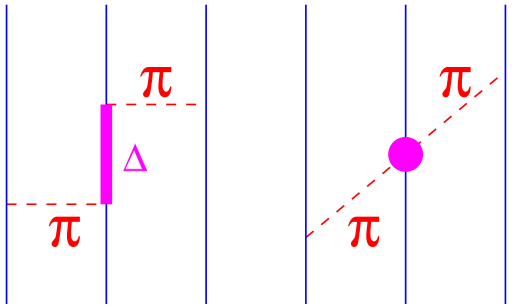
In $A \geq 3$ systems, there is an important 3-nucleon interaction that provides a large fraction of the binding energy

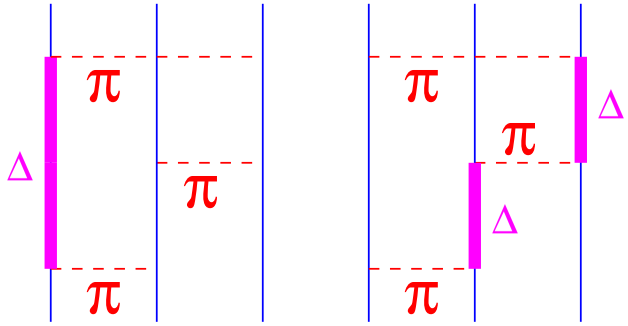
Physically, this arises from lack of explicit π and Δ d.o.f. in the wave function and is tangled with off-shell behavior of NN interaction

NNN interaction is more difficult to constrain than NN because there's no analogue of NN scattering to isolate it

We use (mostly) the Illinois 2 (IL2) NNN interaction:

- 4 terms, spatial/spin/isospin dependence fixed by 2- & 3-pion exchange
- only 4 adjusted parameters (strengths of those terms)
- fixed by fit to 17 bound and narrow levels at $A \leq 8$
- RMS deviation of 700 keV from 60 experimental states in $A \leq 10$





What we actually do, part II: Methods

Variational Monte Carlo (VMC) is built on a sophisticated Ansatz for the wave function, built on shell-model-like structure modified by operator correlations:

Ψ_T = [3-body operator functions] $\times$ [2-body operator functions]
$\times$ [scalar functions] $\times$ [shell-model-like orbital/spin/isospin structure]

Two-body correlations solve sets of differential equations built on the potential, three-body based on 1$^{\text{st}}$-order perturbation

Each piece contains adjustable parameters

We evaluate $E_T = \dfrac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$, a variational bound on ground state energy for given J^π and isospin

We change the parameters by hand, re-compute E_T, and minimize E_T to obtain improving approximations to the ground state and its energy

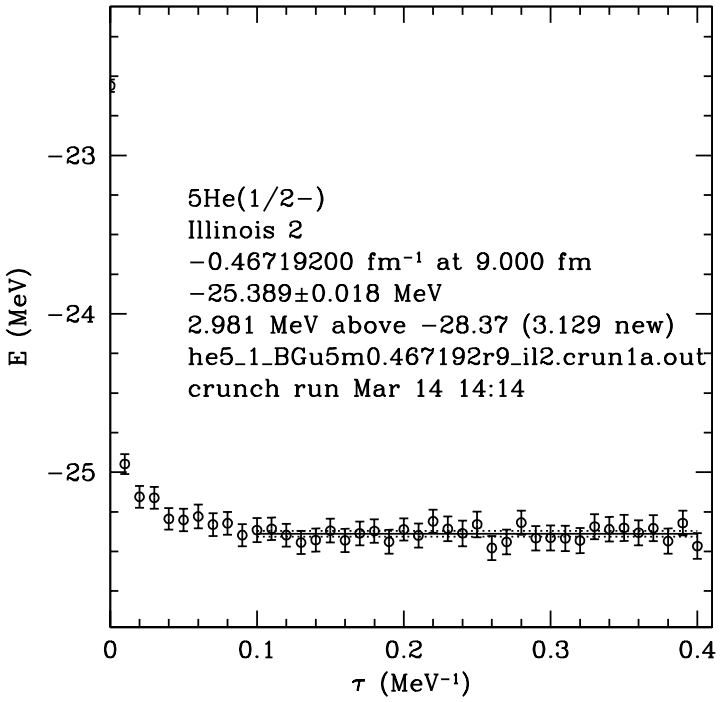
What we actually do, part II: Methods

Green's function Monte Carlo (GFMC) uses an operator method to project the true ground state out of a reasonable guess wave function

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

Ψ_T comes from VMC – a good guess is vital to fast convergence

As $\tau \to \infty$, $\Psi(\tau)$ approaches the ground state



What we actually do, part II: Methods

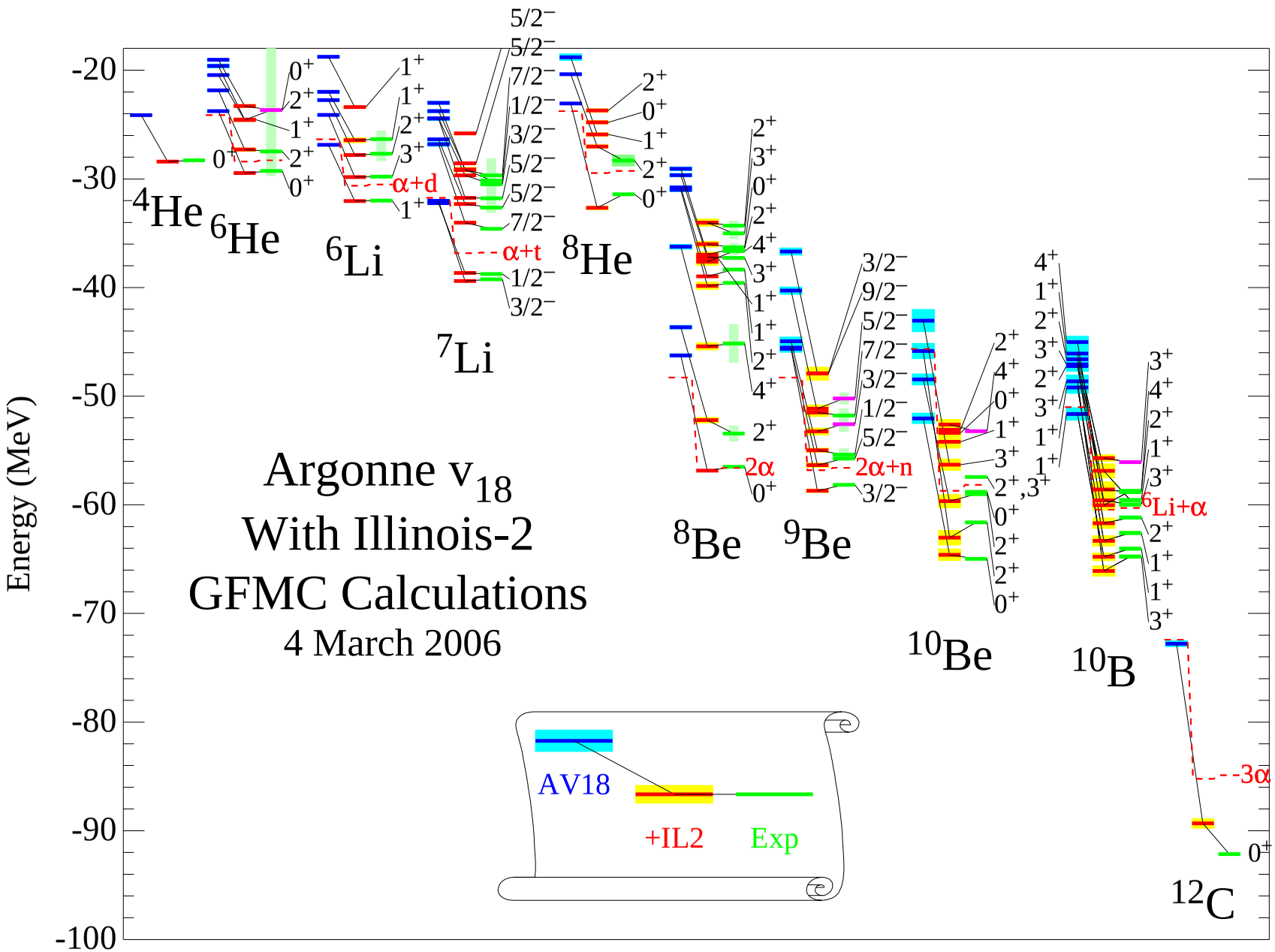
We construct the operator $\exp\left[-\left(H-\tilde{E}\right)\Delta\tau\right]$ as an integral over a Green's function and evaluate its effects by Monte Carlo integration

Result is $\Psi(\tau)$ sampled at discrete points in the particle coordinates

Expectation values are then approximated by $\langle\Psi_T|\mathcal{O}|\Psi(\tau)\rangle$ and corrected perturbatively to obtain $\langle\Psi(\tau)|\mathcal{O}|\Psi(\tau)\rangle$

$\langle H\rangle$ does not have this issue since H commutes with $\exp\left[-\left(H-\tilde{E}\right)\tau\right]$

We have examined quite a large number of bound and narrow states using this method


Energy (MeV)
-20
-30
-40
-50
-60
-70
-80
-90
-100
Argonne v18
With Illinois-2
GFMC Calculations
4 March 2006
4He
6He
6Li
7Li
8He
8Be
9Be
10Be
10B
12C
α+d
α+t
2α
2α+n
6Li+α
3α
AV18
+IL2
Exp

Beyond breakfast (apologies to the Florida orange growers)

Actually, wave function properties beyond bound-state energy levels have been computed for a long time, despite my talk title

However, energy spectra have been emphasized, and emphasis is now shifting to other properties for several reasons

Things that have been computed in the past (and will continue to be computed):

- β decay rates from VMC
- $(e, e'p)$ from VMC
- DWBA overlaps for transfer reactions from VMC
- spectroscopic overlaps from VMC
- RMS radii from GFMC
- radiative capture cross sections from VMC

RMS radii

RMS radii of wave functions can be extracted from GFMC calculations

An initial round of ^{A}He RMS radii turned out to be unconverged due to propagation near edge of 3-D interpolation grid for propagator

After improvement (Pieper and Carlson), found ^{6}He RMS radius good to 1%

Subsequent improvements in Ψ_T made 0.5 MeV change in ^{8}He binding energy

As a result, a re-fitted NNN interaction was needed for RMS radii of weakly-bound states because they are very sensitive to separation energies

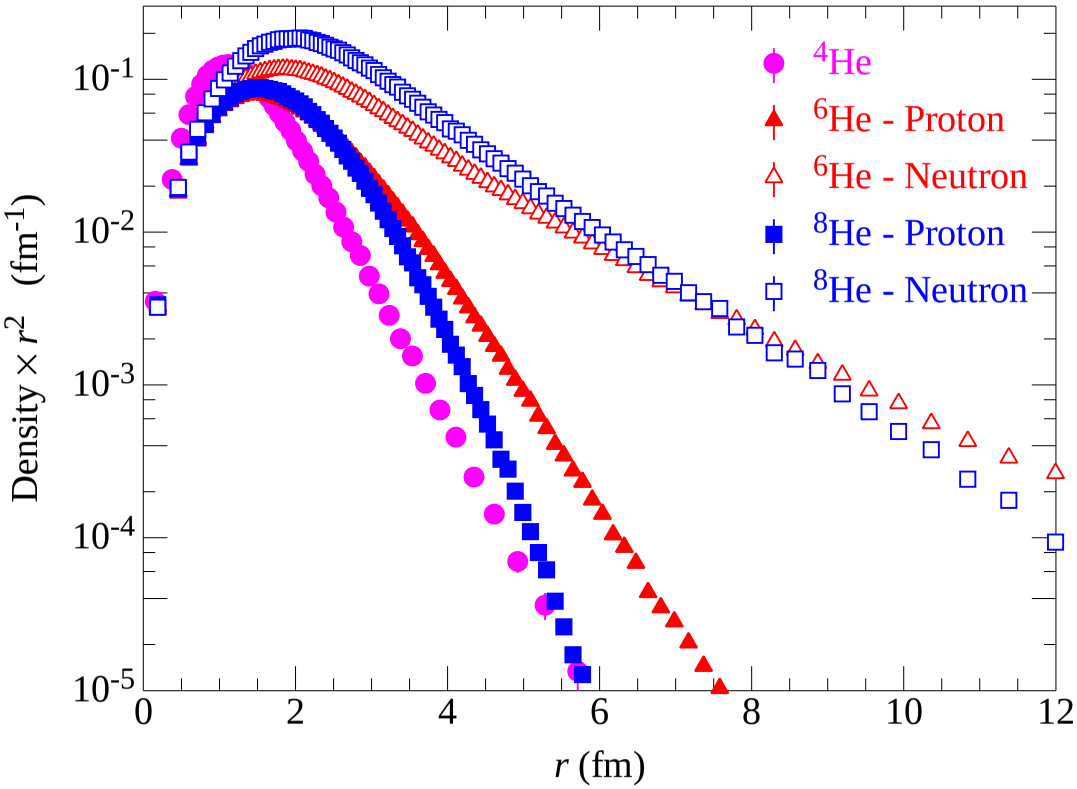
Adjusting two of the IL2 strength parameters by $< 10\%$ gives Illinois 6 and better match to experimental energies in several nuclides

RMS radii

Current batch of **PRELIMINARY** RMS radii:

Point RMS proton radius (fm)

	IL2	IL6	EXPT
^{3}H	1.59	1.60	1.59(5)
^{3}He	1.76	1.76	1.75(1)
^{3}He	1.76	1.76	1.75(1)
^{4}He	1.44	1.45	1.45(1)
^{6}He	1.92	1.95	1.91(2)
^{8}He	1.76	1.79	coming
^{6}Li	2.49	2.49	2.38(3)
^{7}Li	2.30	2.33	2.25(3)
^{8}Li	2.09	2.13	2.16(3)
^{9}Li	2.05		2.08(4)



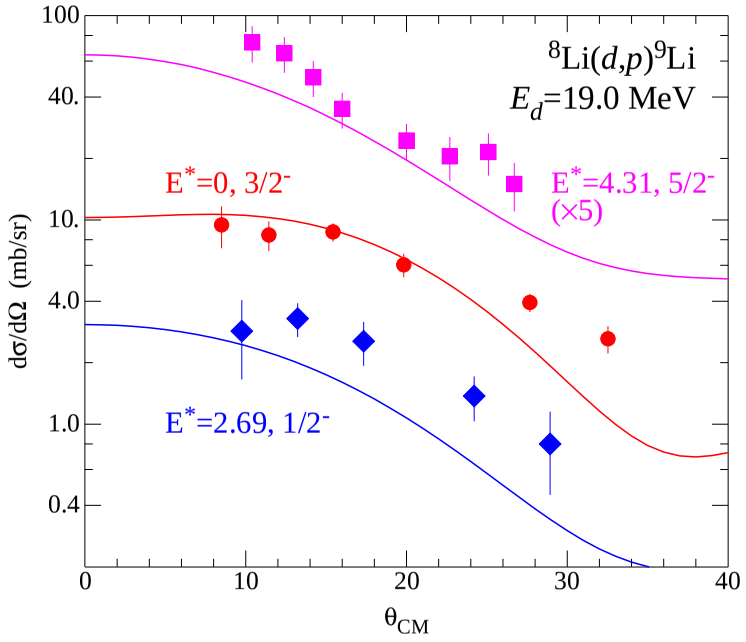
Pickup and stripping

Quantum Monte Carlo and realistic interactions can provide well-motivated vertices and overlaps for DWBA analyses of reactions

With studies of nuclei far from stability, there is new interest in (d, p) and related probes of nuclei

Pieper & Wiringa have contributed to ATLAS radioactive beam experiments on ^{8}Li(d,p)^{9}Li & ^{6}He(d,p)^{7}He

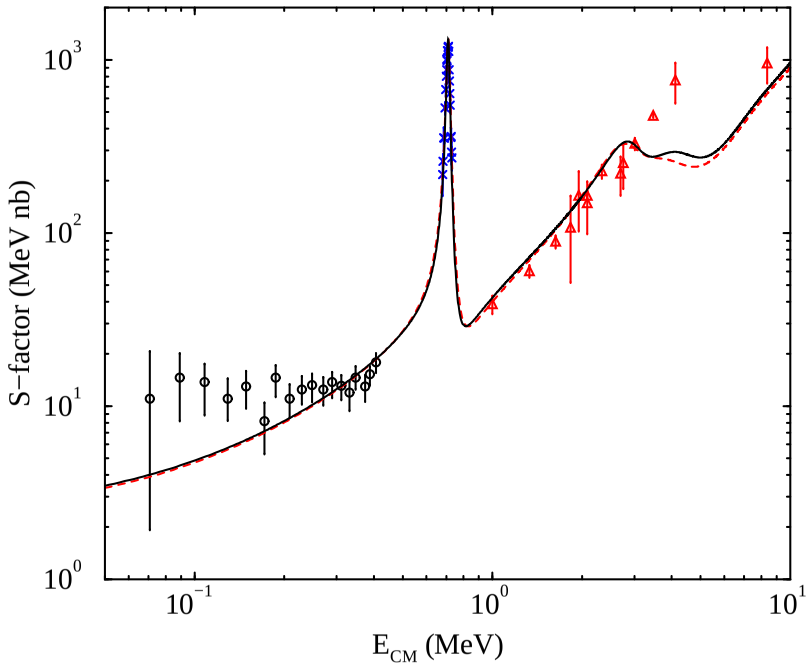
- PTOLEMY DWBA calculations
- (d,p) vertex from Argonne v_{18}
- (^{8}Li,^{9}Li) & (^{6}He,^{7}He) computed as A-body overlaps using VMC $\langle \Psi_T(A) | \Psi_T(A-1) \rangle$; norm is spectroscopic factor
- Strong rejection of previously claimed 560 keV $\frac{1}{2}^-$ state in ^{7}He



Radiative capture

A few years ago, we computed (α, γ) cross sections for astrophysics, using VMC wave functions for bound states and phenomenological prescription for correlations between initial-state nuclei

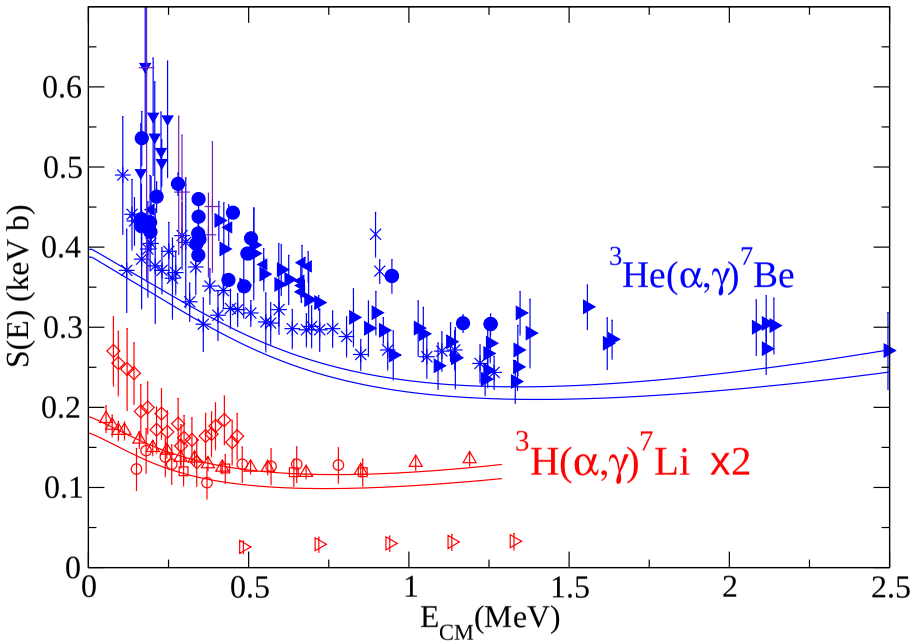
$d(\alpha, \gamma)^6\mathrm{Li}$



Good agreement with direct/low-energy data; disagreement where data are indirect or $T = 1$ channels needed in model

Radiative capture

And more cases (including inconsistent data):



Moving on to reliable, predictive calculations will require:

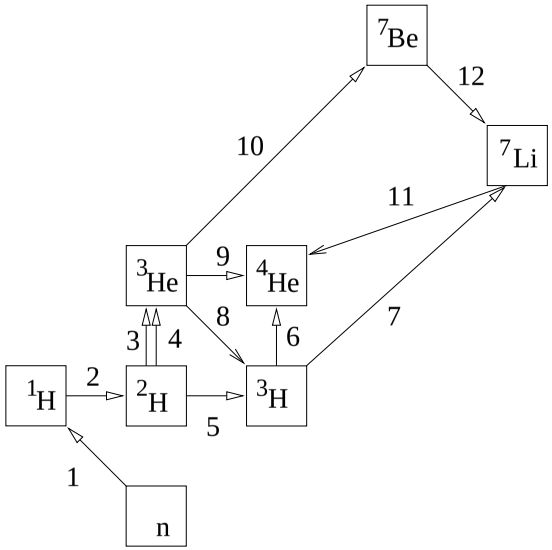
1. whole wave function derived from NN+NNN interaction
2. GFMC wave functions for better accuracy

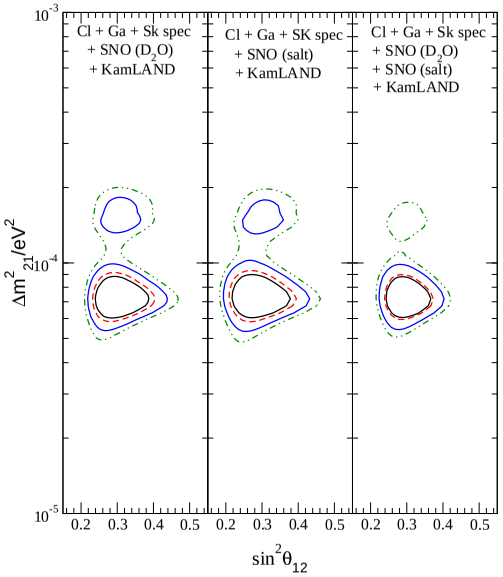
We are now developing methods to treat scattering and address Nos. 1 & 2 at the same time

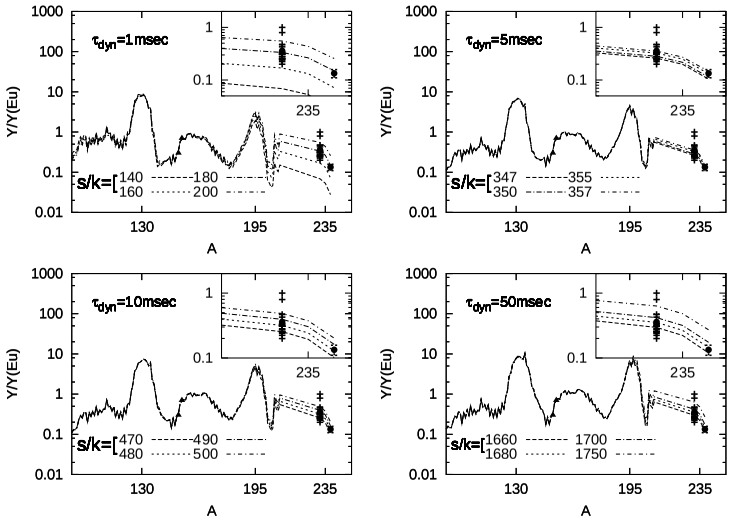
Radiative capture

A reliable treatment of scattering & reactions would open a wider range of experimental tests

It would also provide predictions of absolute cross sections free of convergence difficulties and spectroscopic factor ambiguities
– good for big-bang nucleosynthesis, solar neutrinos, r-process







Newly-completed learning problem: Low-energy ^{4}He+n scattering

Our approach to scattering works like this:

- confine the system to a box with maximum $r_{\alpha n} = R$
- enforce a logarithmic derivative $B = (\hat{\mathbf{n}} \cdot \nabla_{\alpha n} \Psi)/\Psi$ across the surface
- compute energy for the boundary condition
- match across the boundary to free waves to find phase shift δ
- vary B to map out $E(B) \longleftrightarrow \delta(E)$

Easy to implement in VMC, though with limited accuracy

GFMC requires development of techniques to enforce the boundary condition; we use a method of images that is straightforward in ^{5}He case and seems to work well

The quest for accuracy

Low-energy scattering is a demanding problem because we are interested in energy relative to ^{4}He ground state, not absolute energy

Scattering at $E_{\alpha n} = 100$ keV requires $0.100/28.3 = 0.3\%$ accuracy in ^{5}He energy (and ^{4}He energy, but that's easier to get)

At this level, dependence on the starting wave function Ψ_T is noticeable

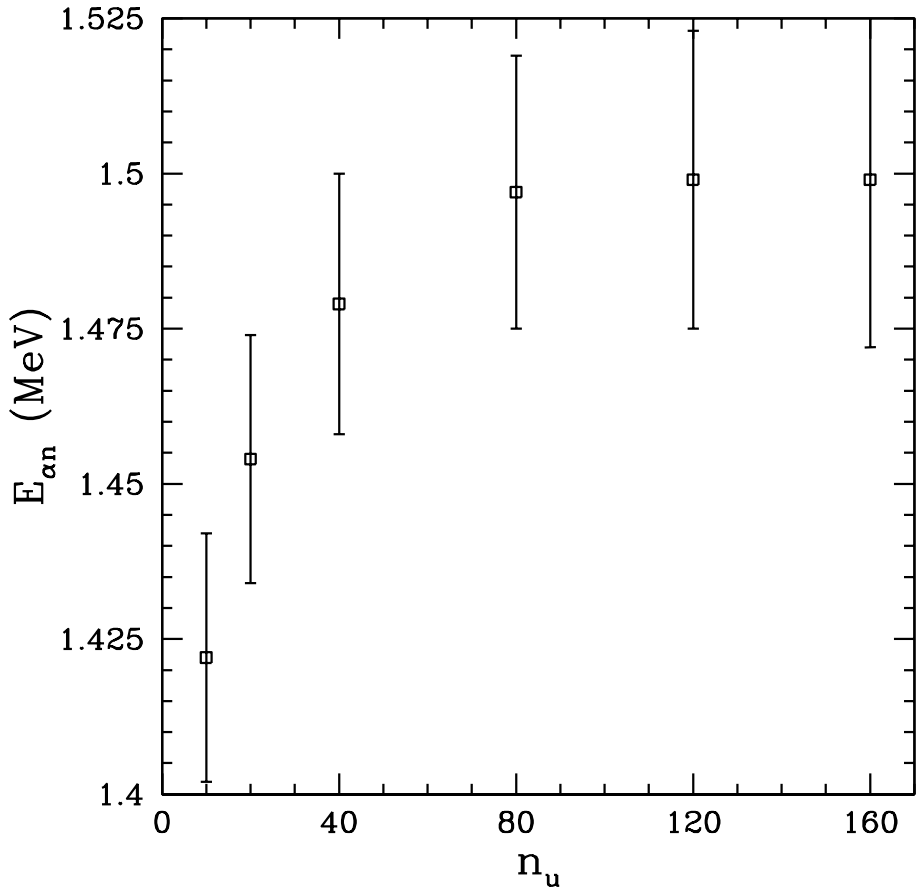
We found that we can decrease this sensitivity by cutting off correlations in Ψ_T beyond the size of ^{4}He and by iteration on a parameter in Ψ_T that governs the ^{4}He+n wave function at large neutron separation

There is also sensitivity to the Monte Carlo path constraint used to avoid the fermion sign problem in GFMC

The constraint eliminates samples that cancel in the final energy calculation, but it can also bias the result

The quest for accuracy

We have always dealt with the bias by removing the constraint for the final $n_u = 10$ to 40 steps in τ

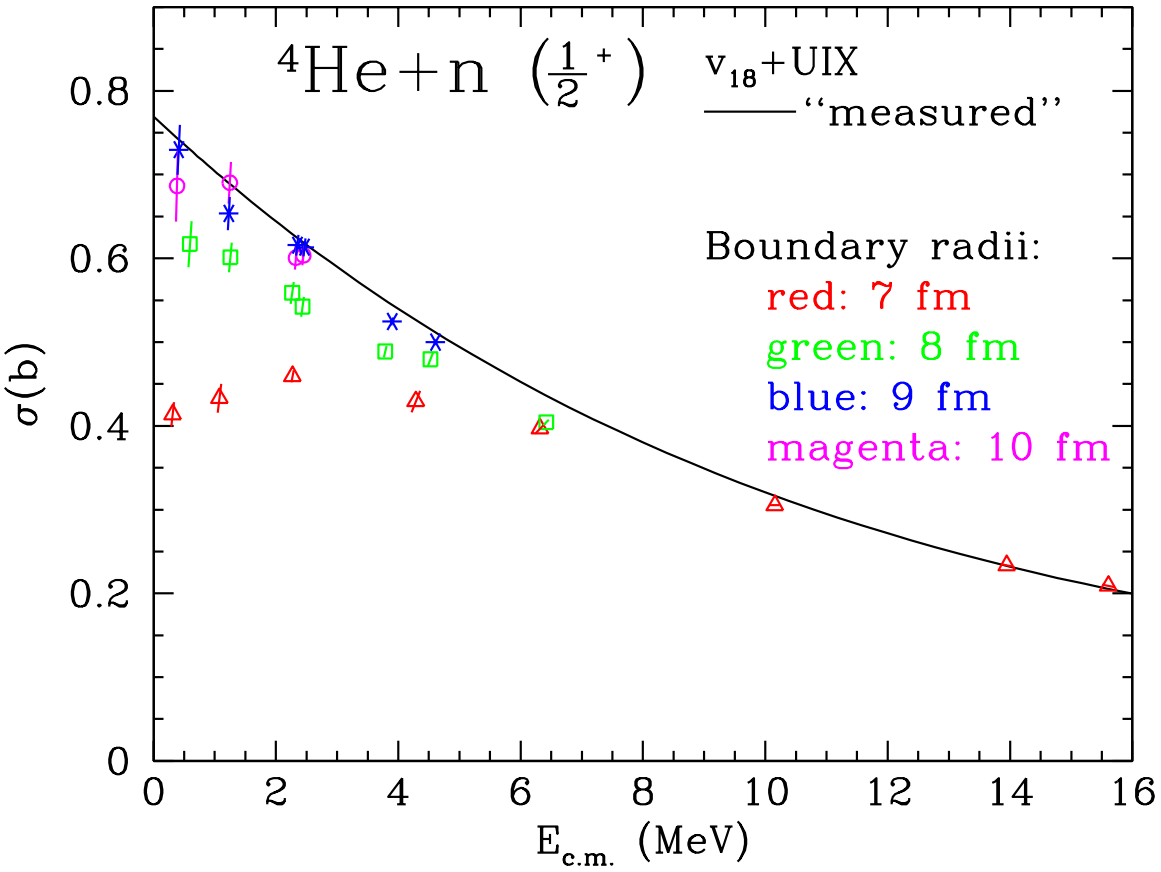


The scattering problem, probably because the wave functions are more diffuse, turned out to need $n_u \geq 80$

The quest for accuracy

The box radius R must be located beyond any interaction between ^{4}He and scattering neutron

But the farther out it is, the less of the box volume is “interesting” and the lower the maximum energy we can compute

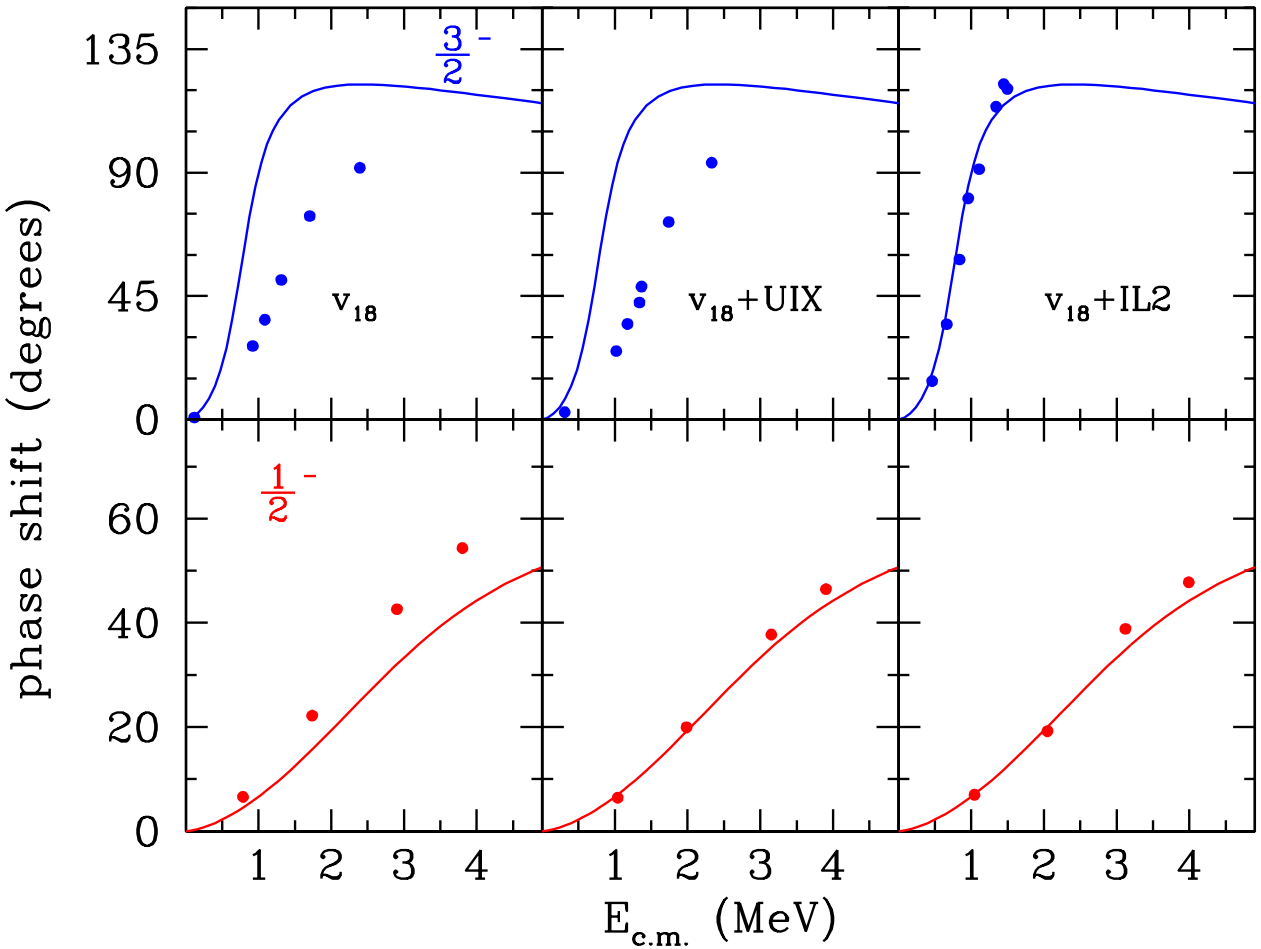


$R = 7$ fm is not large enough

$R = 9$ fm is large enough

^{5}He results

We gain some understanding of spin-orbit splitting of $3/2^-$ and $1/2^-$ resonances

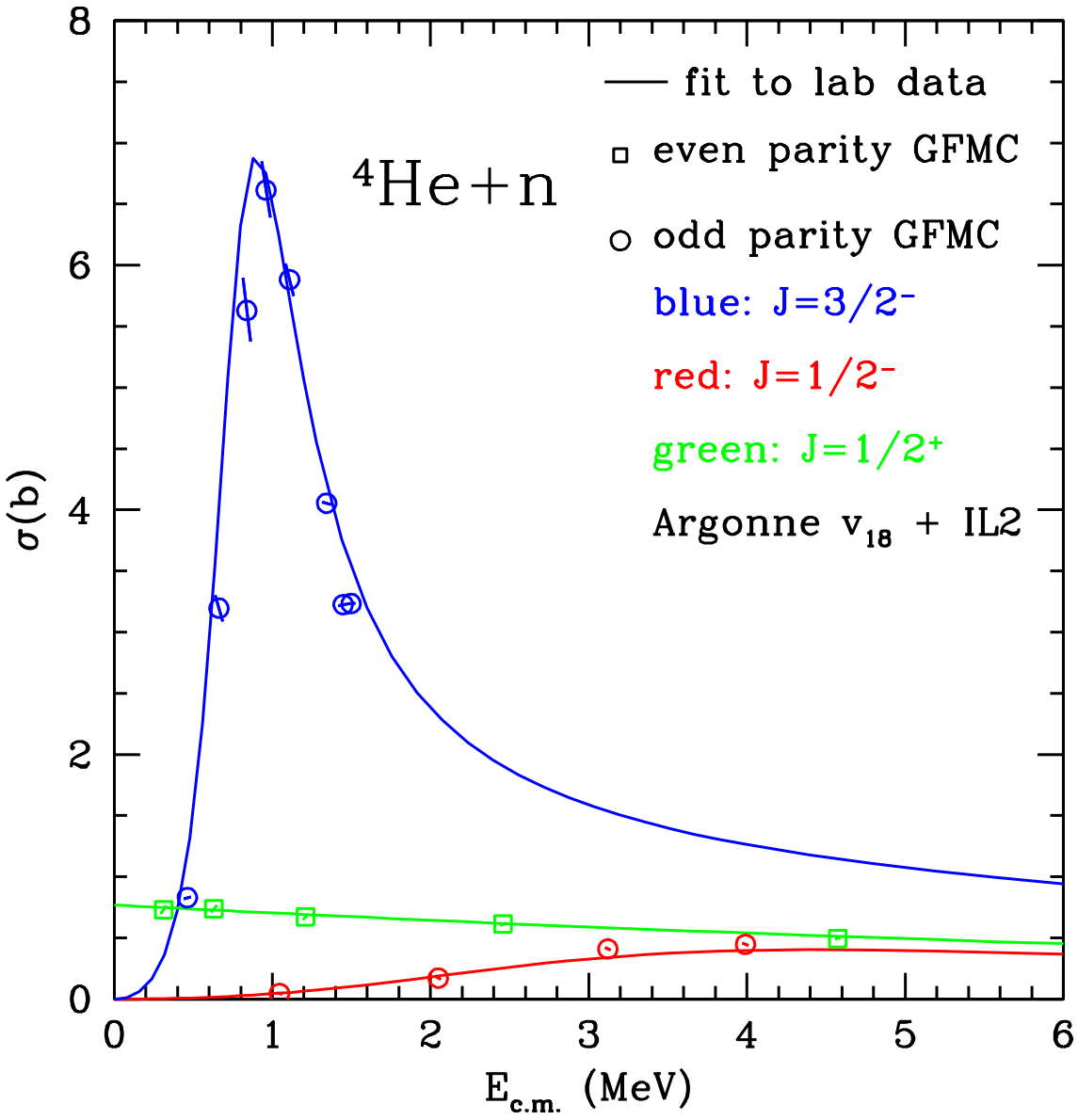


These are also the first-ever calculations of resonance widths in GFMC

(UIX is a previous-generation NNN interaction)

^{5}He results

And overall, v_{18}+Illinois 2 performs embarassingly well



No adjustable parameters!

Directions for the future

There are many further tests and applications of nuclear quantum Monte Carlo and realistic interactions in the near future

Many of these involve radioactive beam experiments and nuclei far from β stability

- astrophysical capture & probably transfer reactions
- study of broad resonances by scattering methods
- easier description of weakly-bound nuclei than in harmonic-oscillator basis
- description of systems with few or no bound states by scattering methods
- anchor for methods that go to higher mass
- launching point for auxiliary-field diffusion Monte Carlo (AFDMC) that replaces explicit spin-isospin sums of GFMC with random sampling to allow larger A
- β decay lifetimes in e.g. ^{8}He, ^{8}B, ^{8}Li, ^{9}C, ^{10}C...

In short, quantum Monte Carlo with bare interactions is well suited to many challenges that are ripe to be taken up, especially in a future that includes radioactive beams

Perhaps most importantly for this meeting, it is preferable to have theory and experiment advance in parallel so that theory can predict outcomes of experiments not yet done

That keeps us honest and also makes the whole enterprise more exciting