Scattering and reactions
in
Quantum Monte Carlo

Ken Nollett
Argonne
23 July 2004
p-shell workshop

It would be nice if nuclear properties could be predicted with confidence from basic principles, particularly for astrophysical problems where the process of interest is unmeasurable or only measurable with substantial effort

QCD is certainly not going to deliver such an understanding of nuclei anytime soon

As a result, astrophysics is dependent on nuclear models that are either built on systematics of many systems and extrapolated to other systems, or ad hoc models that fit properties of a single system (e.g. binding energies, quadrupole moments) in hopes of reproducing its other properties (e.g. cross sections) of the same system

This will always be true

In light systems, at least, there is the potential (no pun!) for predictions from underlying knowledge – models rather than fits – without recourse to interactions fitted to each new problem, poorly-understood effective charges, etc.

Luckily, small-A systems correspond to interesting astrophysics:

big bang
stellar hydrogen burning
solar neutrinos

Realistic potentials

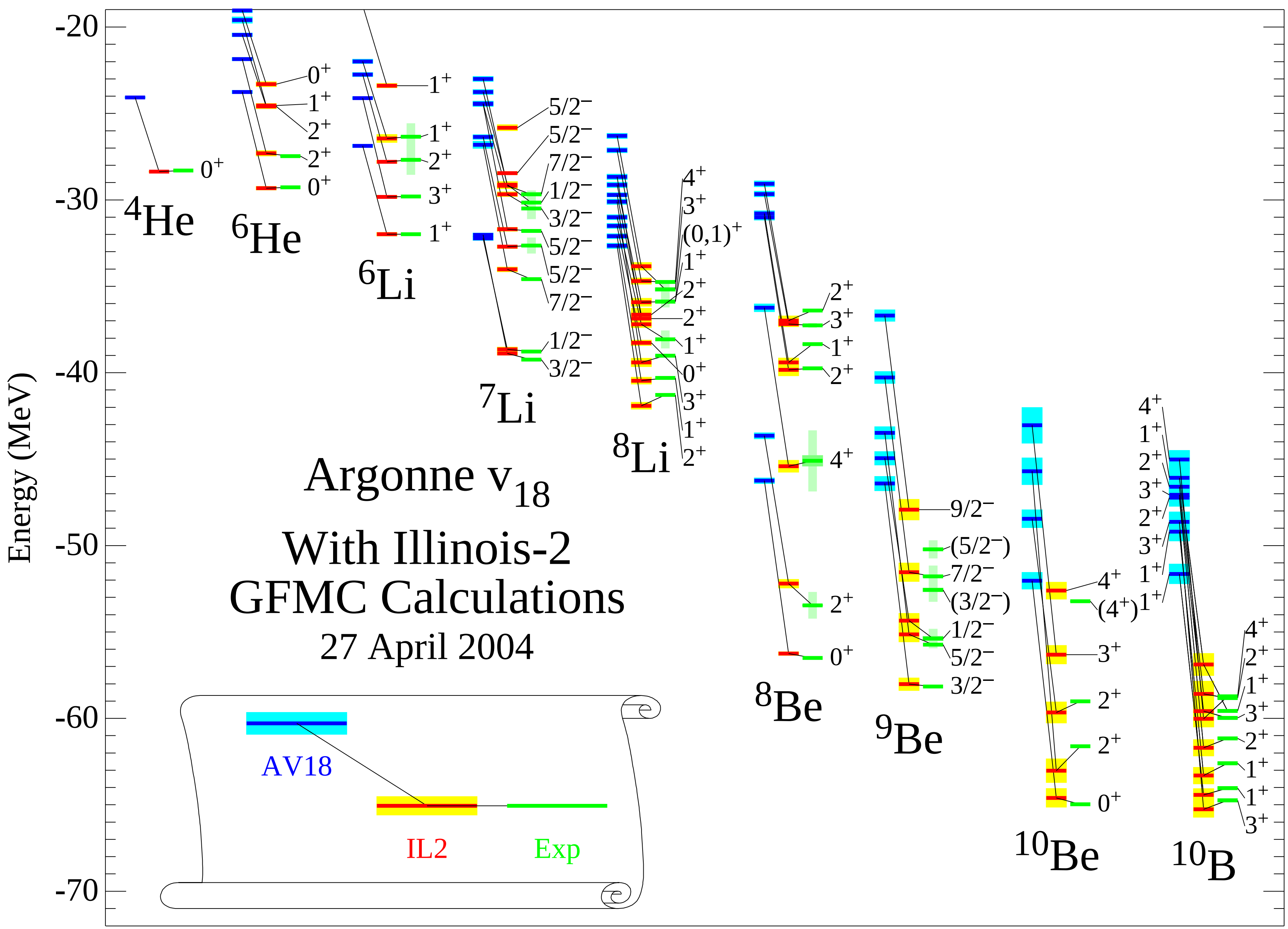
You have already heard a lot about the realistic potentials

I will be talking about wave functions computed using Argonne v_{18} and Urbana IX, extensions and applications of the VMC wave functions Bob Wiringa talked about yesterday

For now, applications will be limited to radiative captures and elastic scattering

Ultimately, we need to switch to Illinois 3-body potentials soon

You probably don't need to be reminded that much of the energy spectrum of light nuclei can be reproduced with these interactions...



Argonne v_{18}

With Illinois-2

GFMC Calculations

27 April 2004

Pieces of a radiative capture cross-section calculation:

$$H\Psi = E\Psi$$

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

Ψ is vector (entry for each permutation of spin and isospin)
function of $3A$ particle coordinates

Solve for initial state Ψ_i with $E > 0$ and final state Ψ_f
with $E < 0$

Cross section is:

$$\sigma^\gamma(E) = \frac{2\,\alpha}{v}\frac{q}{1+q/m_A}\frac{1}{(2J_1+1)(2J_2+1)} \times \sum_{l\geq 1}\sum_{LSJ}\left[\,|\,E_l(q;LSJ)\,|^2 + |\,M_l(q;LSJ)\,|^2\,\right]$$

for EM processes and analogous for weak

$E_l(q;LSJ)$ is one (Wigner-Eckart-reduced) term in multipole
expansion of electromagnetic current matrix element,
$\langle\Psi_f|\mathcal{O}_l|\Psi_i\rangle$

$\langle\Psi_f|\mathcal{O}_l|\Psi_i\rangle$ is inner product in spin-isospin and integral
over all positions

Realistic forces have been applied to several interesting processes in s-shell nuclei by CHH method (Pisa group), or direct solution in $A = 2$:

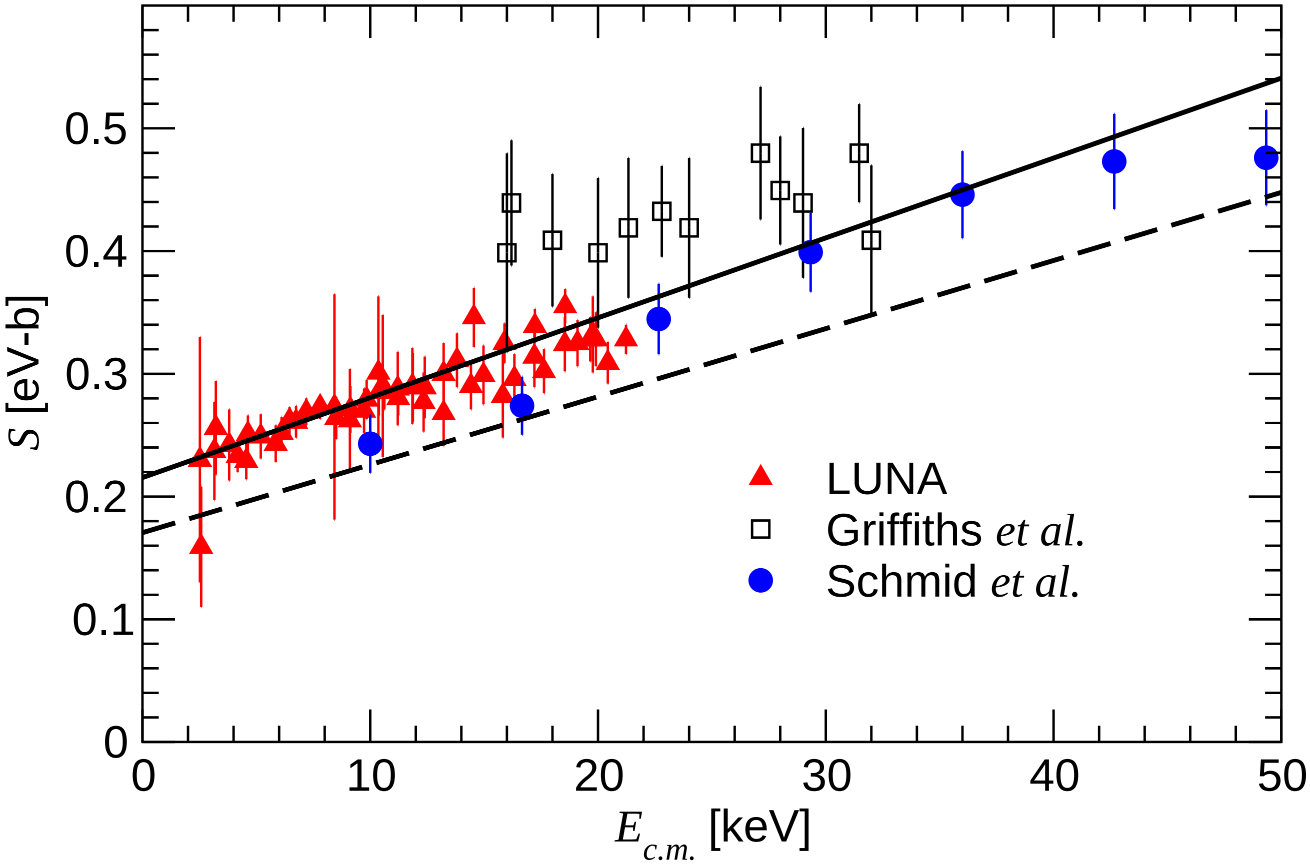
1. $p + p \longrightarrow d + \nu_e + e^+$	sun
2. $p + n \longrightarrow d + \gamma$	big bang
3. $d + n \longrightarrow {}^3\text{H} + \gamma$	method test
4. $d + p \longrightarrow {}^3\text{He} + \gamma$	sun, big bang
5. ${}^3\text{He} + p \longrightarrow {}^3\text{He} + \nu_e + e^+$	sun
6. ${}^3\text{He} + n \longrightarrow {}^4\text{He} + \gamma$	method test

Note that 1 & 5 will never be measured (cross section far too small), so a predictive theory is essential

On 2 and 4, astrophysics needs theoretical input to fill in gaps in the data

Results were mostly successful:

$d(p,\gamma)^3$He – destroys D during big bang



Viviani et al. PRC 61, 064001 (2001)

But some problems remain:

- $d(n,\gamma)^3$H misses by 12%
- ^{3}He$(p,\nu e^+)^4$He neutrino flux is hard to square with computed rate

p-shell final states with variational Monte Carlo

Shell model-like form, product with central operator correlations

$$|\Psi_V\rangle = \left[1 + \sum_{i<j<k\le A} U_{ijk}^{TNI}\right]\left[\mathcal{S}\prod_{i<j\le A}(1+U_{ij})\right]|\Psi_J\rangle$$

$$\begin{aligned}|\Psi_J\rangle = \ & \mathcal{A}\{\prod_{i<j<k\le 4} f_{ijk}^{c} \prod_{i<j\le 4} f_{ss}(r_{ij}) \\ & \times \sum_{LS[n]} \Big(\beta_{LS[n]} \prod_{k\le 4<l\le A} f_{sp}^{LS[n]}(r_{kl}) \\ & \times \prod_{4<l<m\le A} f_{pp}^{LS[n]}(r_{lm})|\Phi_A(LS[n]JMTT_z)_{1234:5\ldots A}\rangle\Big)\ \}\end{aligned}$$

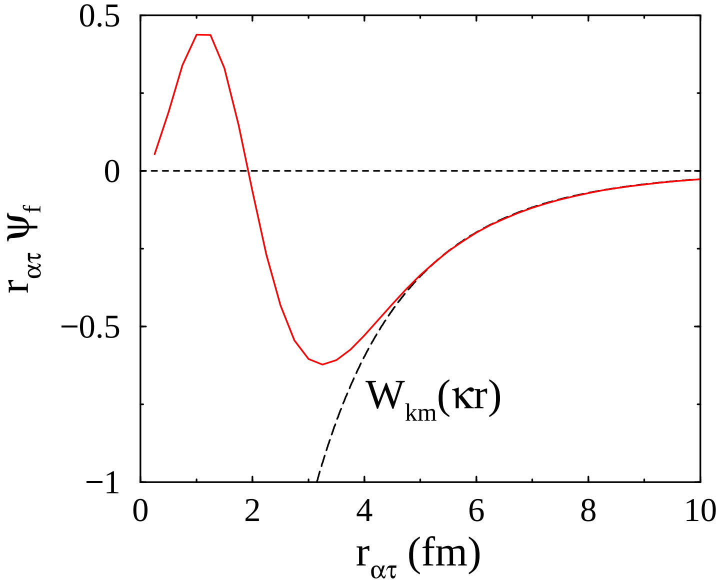
$$\begin{aligned}|\Phi_A(LS[n]JMTT_z)_{1234:5\ldots A}\rangle = |\Phi_4(0000)_{1234}\rangle \\ \times|\textstyle\prod_{4<l\le A}\phi_p^{LS[n]}(R_{\alpha l}) \\ \times\left\{[\textstyle\prod_{4<l\le A} Y_{1m_l}(\Omega_{\alpha l})]_{LM_L[n]} \times [\prod_{4<l\le A}\chi_l(\tfrac{1}{2}m_s)]_{SM_S}\right\}_{JM} \\ \times[\textstyle\prod_{4<l\le A}\nu_l(\tfrac{1}{2}m_t)]_{TT_z}\rangle\end{aligned}$$

Functions based on Hamiltonian plus hand-varied parameters to minimize $\langle H\rangle$

The Ansatz has some limitations – this is why we also use GFMC

Besides providing GFMC initial guess, VMC wave functions are easier to work with in reaction/decay calculations

For low-energy charged-particle capture into weakly-bound states, wave function asymptotics are crucial



Initial-state Coulomb barrier makes much of matrix element arise at large separation

In ^{6}Li, ^{7}Li, ^{7}Be, we modified the single-particle functions $\phi_p^{LS[n]}(R_{\alpha l})$ from bound p-wave asymptotics to

$$\left(\phi_p^{LS[n]}(R_{\alpha l})\right)^{n_p} \propto W_{km}(\kappa R_{\alpha l})/r$$

So for p-shell nucleons far from core, wave functions factor into

^{6}Li $\longrightarrow$ αd s- and d-wave
^{7}Li $\longrightarrow$ $\alpha\,^3$H p-wave
^{7}Be $\longrightarrow$ $\alpha\,^3$He p-wave
(plus smaller components)

VMC Continuum

World experience of QMC unbound states is meagre

Have to confine particles in a box, impose boundary conditions at surface by correct choice of Ansatz and Monte Carlo algorithm

Currently computing ^{4}He+n scattering as a learning problem (VMC & GFMC; more on this later)

For alpha-capture calculations, took VMC states for ^{3}H, ^{3}He, ^{4}He, and exact deuteron

Relative motion from real potentials, fitted to reproduce elastic phase shifts

$$\Psi^{LSJM}_{A_1+A_2} = \mathcal{A}\psi^{LSJ}_{12}(r_{12}) \prod_{ij} G_{ij} \Big[[\phi_1 \otimes \phi_2]_S \otimes Y_L(\hat{\mathbf{r}}_{12}) \Big]_{JM}$$

Important features: forbidden bound states
parity dependence

Operators

Electromagnetic & weak current operators

Unltimately, non-relativistic reduction of things like $\bar{\psi}\gamma^{\mu}A_{\mu}\psi$ and weak operators related by CVC

Boilerplate multipole expansion

A few trickier details:

Esp. where approx. selection rules violated (approximate eigenstates, isoscalar E1), “small” corrections can be important

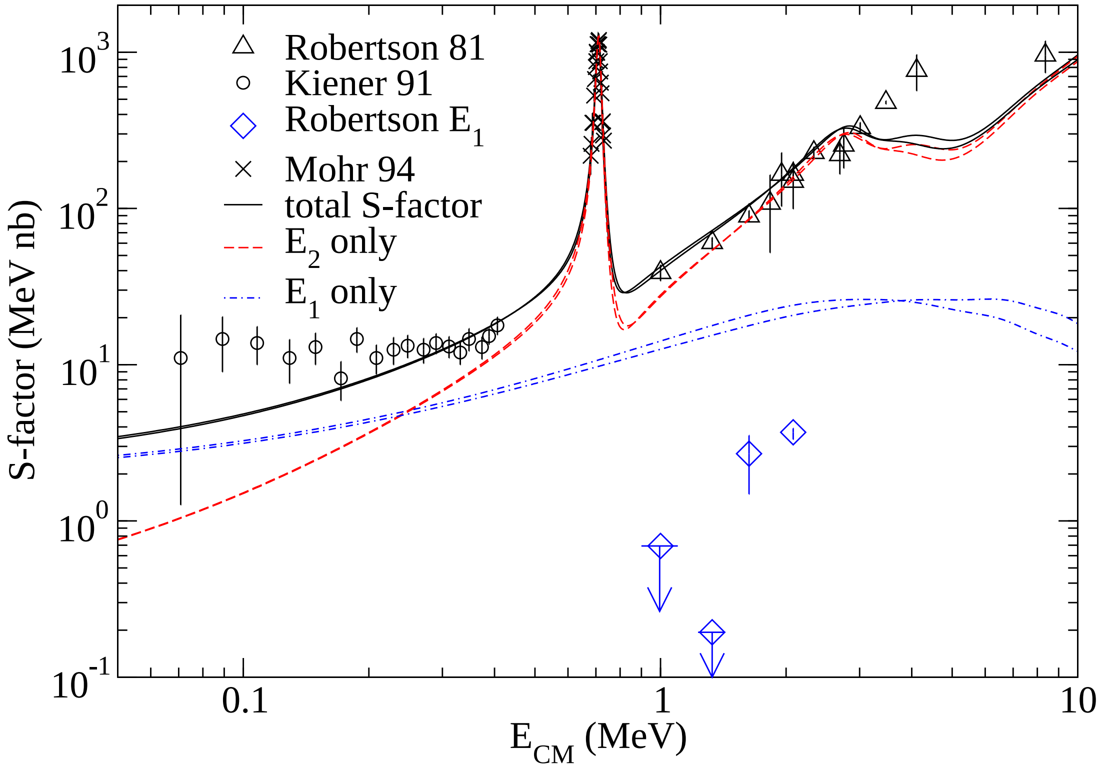
Relativistic & higher-order corrections for $d(\alpha,\gamma)^6$Li isoscalar E1

2-body, Hamiltonian-dependent currents some constrained by charge-conservation & some not

$$\frac{d\rho}{dt} = i[H,\rho] = \nabla \cdot \vec{j}$$

Alpha captures (VMC)

$d(\alpha,\gamma)^6$Li – sets primordial ^{6}Li/H



Nollett, Wiringa, Schiavilla PRC 63, 024003 (2001)

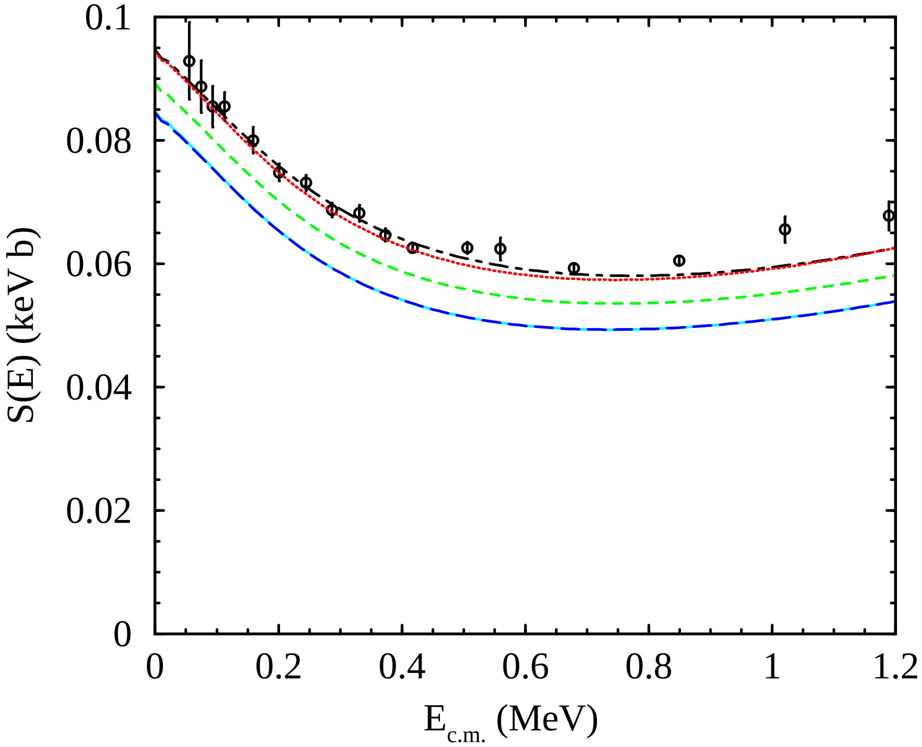
Several small corrections to isoscalar E1 – still get opposite sign from experiment

Note low-E data inferred from Coulomb breakup

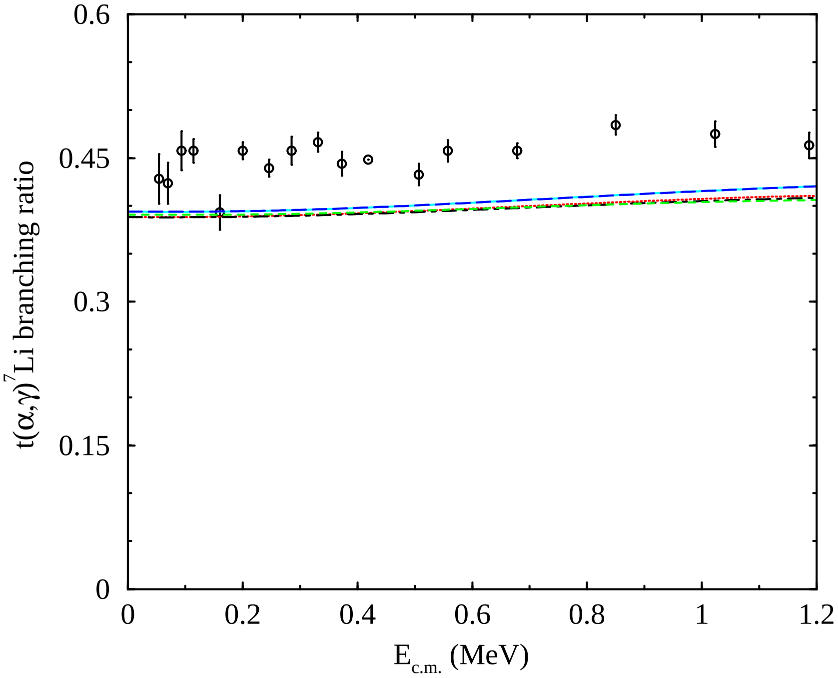
$0 \leq L \leq 3$ in calculation, resonances included in potential model

Mostly $L = 2$, E2 into bound s-wave

^{3}H$(\alpha,\gamma)^7$Li – contributes to primordial ^{7}Li

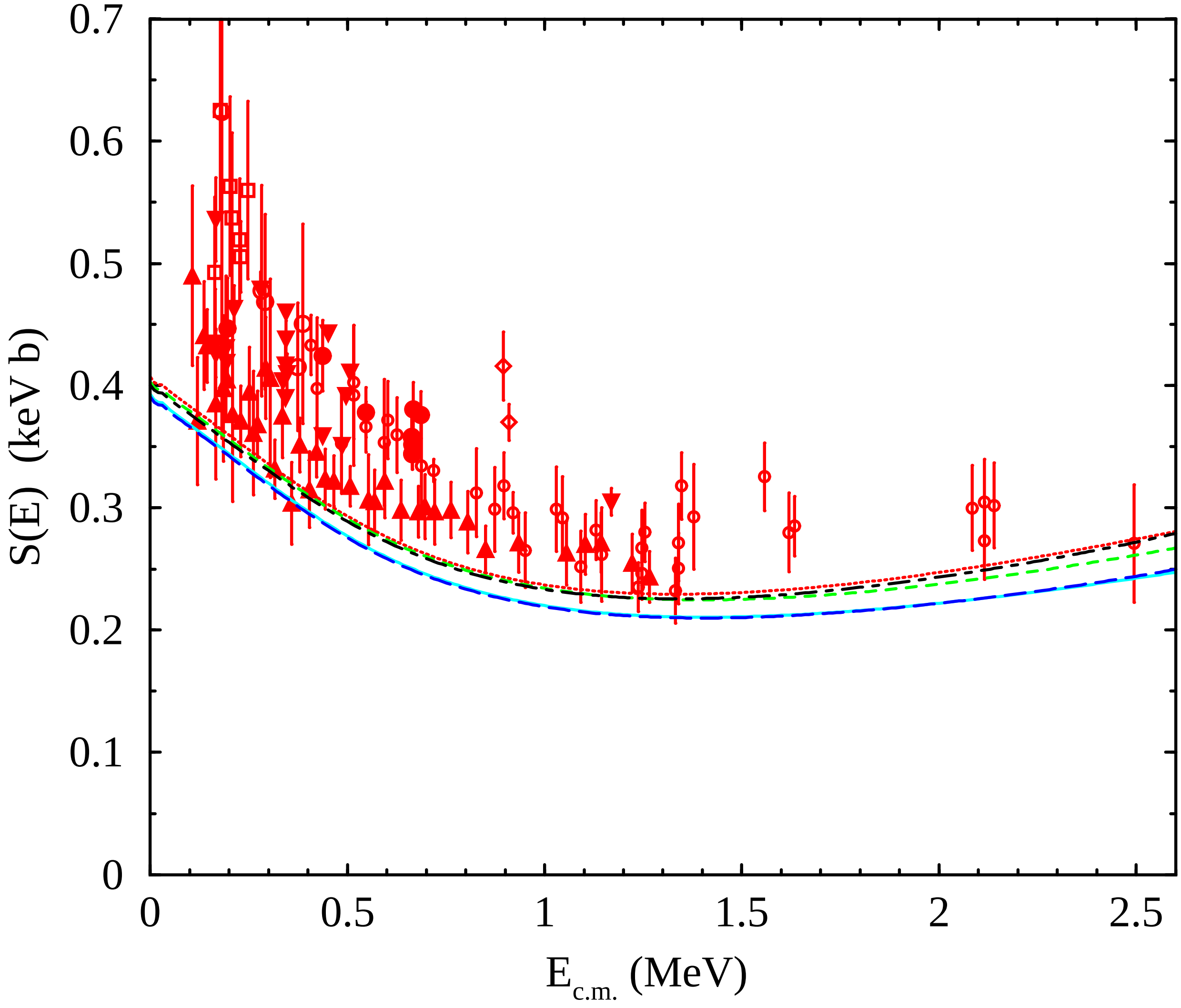


$\chi^2 = 38.7$ for E dependence, 16 d.o.f.



Theory: Nollett PRC 63, 054002 (2001)
Data: Brune, Kavanagh, Rolfs PRC 50, 2205 (1994)

^{3}He$(\alpha,\gamma)^{7}$Be – source of ^{7}Li in big bang
path to solar neutrinos



Nollett PRC 63, 054002 (2001)

Isospin mirror of ^{3}H$(\alpha,\gamma)^{7}$Li

Less dependence on scattering, very similar to other models in literature

As with ^{3}H$(\alpha,\gamma)^{7}$Li, mostly $L=0$, some $L=2$, essentially all E1

What I’ve shown you is just the beginning, more proof of concept than anything

Advances more or less within reach (more detail in a moment):

* QMC scattering states derived from the NN potentials

Connection with R-matrix, scattering data, (transfer reactions?)

* Green’s Function Monte Carlo wave functions

* Gell-Mann-Goldberger method for asymptotics

Illinois NNN potentials

Several more astrophysically interesting reactions, to at least $A = 9$

Asterisks are steps between us and strong predictions of absolute cross sections

Scattering states from quantum Monte Carlo

Obvious place to improve: big part of VMC calculations weren’t based on the potential

Many of Bob’s & Steve’s states are particle unstable narrow states, treated as bound, so it would be good to check them

For nucleus-nucleon scattering, procedure is fairly obvious

Obvious continuum state procedure

1. Restrict Monte Carlo walk so last nucleon is within a specified distance of nuclear center of mass, $r < a$
2. Enforce specified logarithmic derivative of wave function at boundary, $\frac{1}{r\Psi}\frac{d(r\Psi)}{dr} = \frac{B}{a}$
3. Minimize energy E by VMC and/or GFMC
4. Phase shift is a known function of E & B; compare with data
5. Repeat for other B & map out phase shifts as function of E
6. Use results for capture calculations where applicable

In practice, take VMC bound state form that I showed,
replace single-particle correlation of last particle with
a function that enforces log derivative boundary condition

Bound single-particle function:

$$\left[-\frac{\hbar^2}{2\mu_{41}}\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right)+V\right]r\phi_p^{LS}(r)=-Er\phi_p^{LS}(r)$$

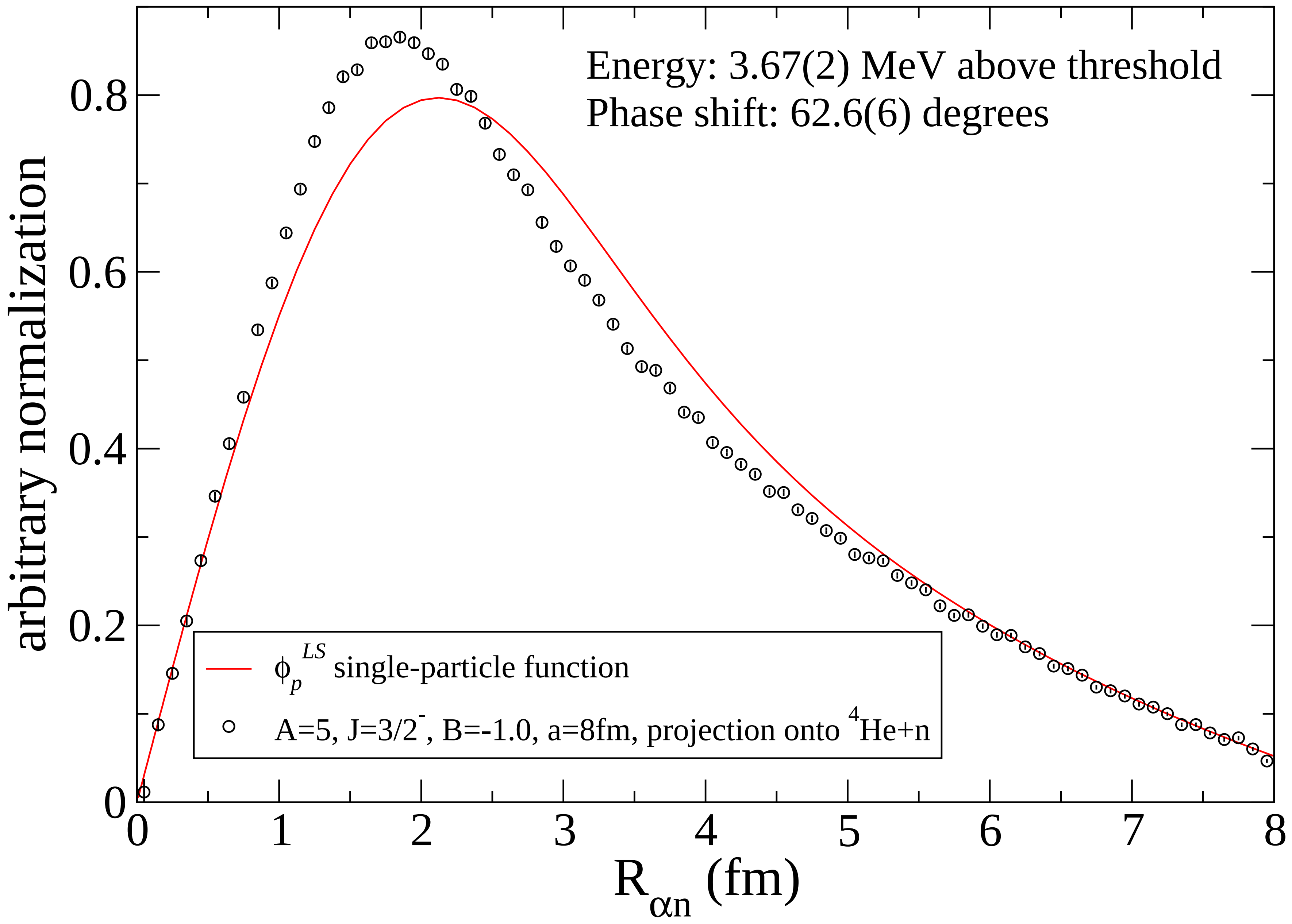
$$V(r)=\frac{V_0}{1+\exp[-(r-R)/a]}$$

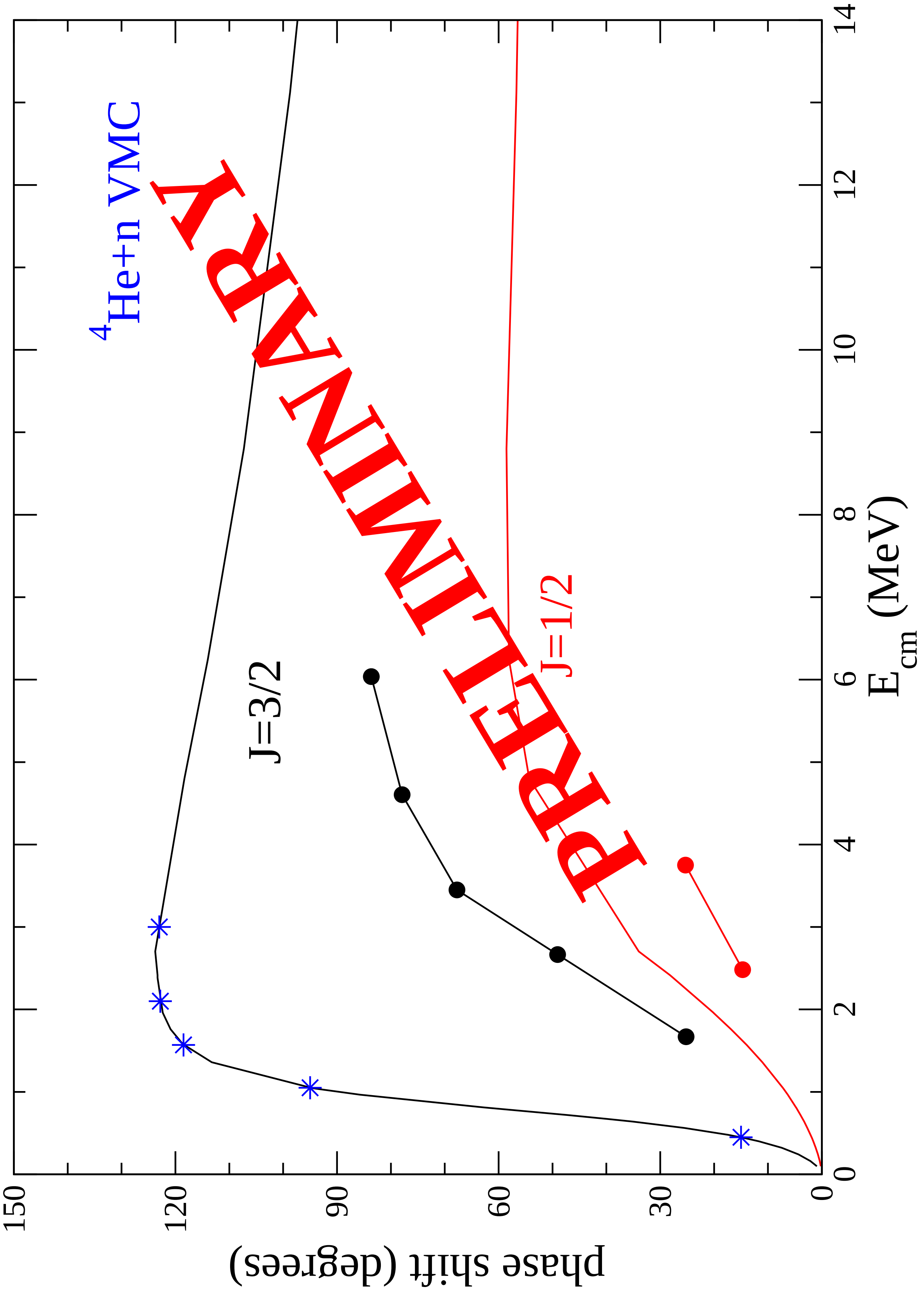
$$r\phi_p^{LS}(r\to\infty)\propto j_1(kr), \qquad k=\sqrt{2\mu E}/\hbar$$

Scattering:

- change boundary condition to $\frac{d}{dr}(r\phi_p^{LS})=\frac{B}{a}(r\phi_p^{LS})$
- make sure all other correlations are 1 at this position
- adjust parameters variationally

I'm currently at work on low-energy scattering in ^{4}He+n


Energy: 3.67(2) MeV above threshold
Phase shift: 62.6(6) degrees
ϕ_p^{LS} single-particle function
A=5, J=3/2$^-$, B=-1.0, a=8fm, projection onto ^{4}He+n
arbitrary normalization
0
0.2
0.4
0.6
0.8
0
1
2
3
4
5
6
7
8
$R_{\alpha n}$ (fm)


⁴He+n VMC
PRELIMINARY
J=3/2
J=1/2
E_cm (MeV)
phase shift (degrees)
0
2
4
6
8
10
12
14
0
30
60
90
120
150

Note the close connection to R-matrix theory:

In R matrix, there is a boundary at $r = a$ outside nuclear interaction radius where wave function log derivative is B

Inside the boundary, Hamiltonian plus boundary conditions define a basis of discrete states with some energy spectrum

At arbitrary energy, interior part of wave function may be expanded in terms of these states by matching to external wave function at a

Scattering properties can be found entirely from energies E_i of interior functions, and their amplitudes γ_i at a

Past application has involved fitting E_i and γ_i to data

We should be able to compute at least the lowest E_i and γ_i from NN interactions

Definitely useful for comparison between theory and scattering data

Potentially useful for efficient capture calculations

Maybe even a door toward transfer reactions?

A big problem in α-captures was sampling in the wave function tails

Tails are where

- most of matrix element integrand is concentrated for low-E captures
- shape (but not amplitude) of wave function is determined completely by energy and (if present) Coulomb barrier

Monte Carlo integration in the tails requires either

1. many more samples (and thus low efficiency because most wave-function-weighted samples go into interior)
2. sampling procedure weighted more for tails but still a good match to other aspects of matrix element density

or

3. combination of 1 & 2

In $A = 6$ capture, that worked. In $A = 7$, it didn't.

We found matrix element densities, e.g. $\langle\alpha\,{}^3\mathrm{He}\,\delta(r_{\alpha 3}-R)|\mathcal{O}_l|{}^7\mathrm{Be}\rangle$, extracted norm at R where wave function was asymptotic, and used that to normalize asymptotic form

Part of integrand beyond matching radius computed from exact function instead of Monte Carlo

Will probably move to applying Gell-Mann-Goldberger theorem relating asymptotic normalization to wave function in interior region:

$$\int_0^a \Psi^\dagger (V - V_C^{12}) \Psi dr_{12} = C$$

That's the sort of thing the Monte Carlo method is good at, and it simplifies assignment (and minimization) of formal sampling error

When these developments, and GFMC wave functions, are applied to radiative capture, we can predict absolute cross sections in $A > 4$ systems with great confidence

Either

We reproduce data where there are reliable data and provide useful new information (e.g., break deadlock on ^{3}He$(\alpha, \gamma)^7$Be)

or

We really learn something about the limits of what we can do

Finally, more reactions can be done or re-done

Reaction	Why	Pre-requisite
^{3}He$(n,\gamma)^4$He	test	scattering states
^{3}He$(\alpha,\gamma)^7$Be	sun,BBN	scattering,GFMC,tails
^{2}H$(\alpha,\gamma)^6$Li	$E1$ puzzle	scattering,GFMC,tails
^{7}Be$(p,\gamma)^8$B	sun	scattering,tails,GFMC?
^{7}Li$(n,\gamma)^8$Li	test	scattering,tails
^{8}Be$(n,\gamma)^9$Be	r process	scattering,tails,GFMC?

Interesting stuff ahead!