Quantum Monte Carlo (QMC) Calculations of n + ^{4}He Scattering

Abraham R. Flores
Washington University in St. Louis

ECT*

June 18th : 2024

Collaborators

Maria Piarulli (WASHU)
Saori Pastore (WASHU)
Bob B. Wiringa (ANL)
Alessandro Lovato (ANL)
Kenneth Nollett (SDSU)

Work Supported by the US Department of Energy, Office of Nuclear Physics Award DE-SC0019257 (K.M.N)
Work Supported by the 2021 Early Career Award No. DE-SC0022002 and the FRIB Theory Alliance Award No. DE-SC0013617 (M.P.)
Work Supported by DOE DE-SC0021027 (S.P.)

The many-body calculations were performed on the parallel computers of the Laboratory Computing Resource Center, Argonne National Laboratory, and the computers of the Argonne Leadership Computing Facility via the INCITE grant "Ab-initio nuclear structure and nuclear reactions.

Current many-body calculations are performed under the support of National Energy Research Scientific Computing Center (NERSC)

Ab Initio Calculations of Nuclear Collisions

Why?

- Predictive theory of all nuclei
  - Reliable predictions of low-energy reaction cross sections

What We Need

- Accurate Two Nucleon interaction (NN)
- Accurate Three Nucleon interaction (NNN)
- Solver for many-nucleon Schrödinger Equation
  - QMC has been successful for bound states up to ^{12}C

What We Want

- Unified treatment of collisions & bound states
- Uncertainty quantification for our choice of nucleon interaction
- Improved NN, NNN models

Nuclear Potentials

Phenomenologically Organized Potentials

Two Nucleon (NN)

- Argonne v_{18}
  - (Wiringa, Stoks, Schiavilla, 1995)
  - 1787 pp scattering data
  - 2514 np scattering data
  - low energy nn scattering parameters
  - deuteron binding energy
  - χ^2 per datum = 1.09
- Also CD Bonn, Nijmegen I & II, Paris...

Three Nucleon (NNN)

- Urbana IX , X
  - (Carlson, Pandharipande, Wiringa, 1994)
  - Two pion exchange contributions
  - ^{3}H , ^{4}He binding energies
- Illinois 7
  - Pieper, Pandharipande, Wiringa, and, Carlson (2001)
  - Urbana + three pion rings
  - Energy levels up to A = 8

Nuclear Potentials

Chiral Potentials

Application of chiral perturbation theory to nuclear interactions (Weinberg, 90,91,92)

Success in organizing and fitting two-body interaction

Three nucleon interaction is a topic of active research

- Idaho (Entem, Machleidt, 2002)
- Darmstadt (Lynn *et al*, 2016)
- **Norfolk (Piarulli *et al*, 2016), (Piarulli *et al*, 2018)**
  - nn, np, pp scattering data
  - χ^2 per datum ~ 1.3
  - 4 two-body versions (e.g. NVIa)
  - 8 two- and three-body versions (e.g. NV2+3Ia)
  - Different choices of data and model space

***QMC methods need a potential that is diagonal in r-space (not momentum-space)**

Scattering Formalism

T-, S-, and K- matrix

$$\mathcal{H}_c^{\pm} = \mathcal{G}_c \pm i\mathcal{F}_c$$

$$\Psi(\text{all } r_c \to \infty) = \sum_c \left(A_c \mathcal{F}_c + B_c \mathcal{G}_c\right) \qquad \mathbf{B} = \hat{K}\,\mathbf{A}$$

$$\Psi(\text{all } r_c \to \infty) = \sum_c \left(\mathscr{A}_c \mathcal{F}_c + \mathscr{B}_c \mathcal{H}_c^{+}\right) \qquad \mathscr{B} = \hat{T}\,\mathscr{A}$$

$$\Psi(\text{all } r_c \to \infty) = \sum_c \left(\alpha_c \mathcal{H}_c^{-} + \beta_c \mathcal{H}_c^{+}\right) \qquad \beta = \hat{S}\alpha$$

These amplitudes encode the scattering information!

Variational Monte Carlo (VMC)

Variational Wave Function

Z = number of protons

A = number of nucleons

Wiringa (1991)

Ψ_V are position dependent spin-isospin column vectors with ~ $2^A \binom{A}{Z}$ components

(two & three body)

$$|\Psi_V\rangle = \{\mathcal{S} \times [\text{operator correlations}]\} \times |\Psi_J\rangle$$

(pairs & triplets)

shell-model-like
orbital / spin / isospin structure

$$|\Psi_J\rangle = \mathcal{A}\{[\text{scalar correlations}] \times \sum_{LS[n]} \beta_{LS[n]} |\Phi_A(LS[n]JMTT_z)\rangle\}$$

Two-body correlations solve sets of differential equations built on the potential

Three-body based on 1st-order perturbation

Each piece contains adjustable parameters

Variational Monte Carlo (VMC)

Wiringa (1991)

MINIMIZE $$E_V = \frac{\langle \Psi_V | \hat{H} | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0$$

High dimensional integrals are done through Monte Carlo integration

Expectation values are integrated by a Metropolis sampling

Optimize parameters to seek lower energies

Generates good approximate wave function for specified quantum numbers

Adapting VMC to Scattering States

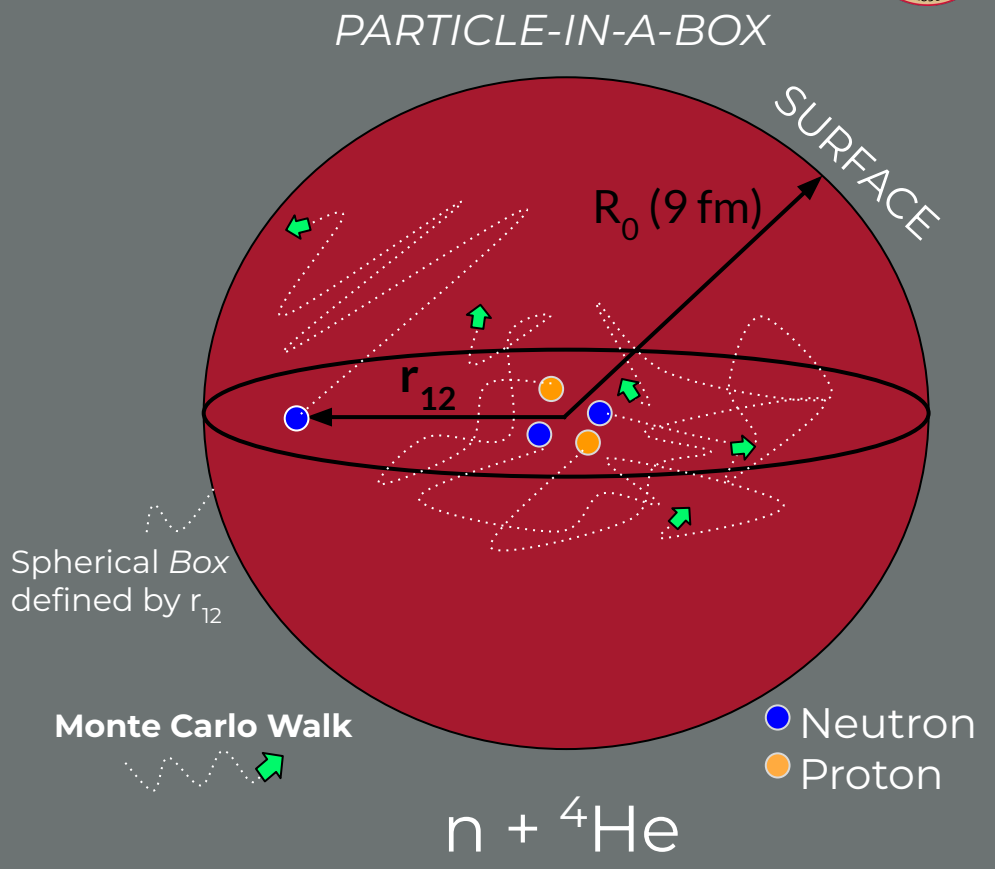
True Scattering Boundary Condition

$$\Psi(\text{all } r_c \to \infty) = \sum_c (A_c \mathcal{F}_c + B_c \mathcal{G}_c)$$

VMC needs an eigenvalue problem

Log-Derivative Boundary Condition

$$\hat{\mathbf{n}}_c \cdot \nabla_{\mathbf{r}_c} \left(\mathbf{r}_c \left| \Psi \right\rangle \right) = \zeta_c \mathbf{r}_c \left| \Psi \right\rangle$$



Single Channel Scattering

match smoothly across the boundary to get

$$\tan\delta = \left.\frac{k\frac{\partial}{\partial\rho}F_l(\eta,\rho) - \zeta F_l(\eta,\rho)}{\zeta G_l(\eta,\rho) - k\frac{\partial}{\partial\rho}G_l(\eta,\rho)}\right|_{\rho=kR_0}$$

Requires boundary condition + Energy

or

$$\tan\delta = \frac{B}{A}$$

Requires surface amplitudes

Surface Amplitudes in VMC

For coupled channel problems there is no choice!

The surface amplitudes must be computed!

VMC ansatz is poor outside the region of interaction

Limited options for optimizing wavefunction at the surface (bad at collectivity)

Incorrect wave function tails are a common symptom in many-body methods

Need a method for computing surface amplitudes that takes advantage of the accurate interior (<5 fm) part of the wave function

Integral Method

(Pinkston & Satchler 65) , (Kawai & Yazaki 67) , (Mukhamedzhanov & Timofeyuk 90) , (Kievsky, 10) , (Nollett 12)

$$G_l \frac{\partial F_l}{\partial \rho} - F_l \frac{\partial G_l}{\partial \rho} = 1 \quad \text{and Green's Theorem}$$

$$\frac{2\mu k_c}{\hbar^2}\left(\langle \mathcal{F}_c| \hat{H} - E |\mathcal{G}_c\rangle - \langle \mathcal{G}_c| \hat{H} - E |\mathcal{F}_c\rangle\right) = 1$$

$$A_c = \frac{2\mu}{\hbar^2}\left(\langle \Psi| \hat{H} - E |\mathcal{G}_c\rangle - \langle \mathcal{G}_c| \hat{H} - E |\Psi\rangle\right)$$

$$B_c = \frac{2\mu}{\hbar^2}\left(\langle \mathcal{F}_c| \hat{H} - E |\Psi\rangle - \langle \Psi| \hat{H} - E |\mathcal{F}_c\rangle\right)$$

For the true wave function $(\hat{H} - E)|\Psi\rangle = 0$

Regularization

Dealing with the irregular coulomb function

divergence in G_l at $r_c = 0$ gives rise to a delta-function in $\nabla^2 G_l$

Difficult to sample zero cluster separation

$$\widetilde{\mathcal{G}}_c = \mathcal{G}_c - f_c(r_c;\gamma)\Psi_{n\otimes\alpha}$$

$$\lim_{r_c \to 0} \widetilde{\mathcal{G}}_c = 0$$

$$\lim_{r_c \to R_0} \widetilde{\mathcal{G}}_c = \mathcal{G}_c$$

*We use the regularizer from Viviani 2020)

Integral Method

(Kievsky, 2010)

$$\frac{2\mu k_c}{\hbar^2}(\langle \mathcal{F}_c| \hat{H} - E |\widetilde{\mathcal{G}}_c\rangle - \langle \widetilde{\mathcal{G}}_c| \hat{H} - E |\mathcal{F}_c\rangle) = 1$$

$$A_c = \frac{2\mu}{\hbar^2}\left(\langle \Psi| \hat{H} - E |\widetilde{\mathcal{G}}_c\rangle - \langle \widetilde{\mathcal{G}}_c| \hat{H} - E |\Psi\rangle\right)$$

$$B_c = \frac{2\mu}{\hbar^2}\left(\langle \mathcal{F}_c| \hat{H} - E |\Psi\rangle - \langle \Psi| \hat{H} - E |\mathcal{F}_c\rangle\right)$$

Integral Method In VMC

$$E_{\rm rel} = E_{\rm tot} - E_\alpha$$

(Flores & Nollett 2023)

If ... $\boxed{(\hat{H}_\alpha - E_\alpha)\,|\Psi_\alpha\rangle = 0}$

$$A_{V,c} \approx \frac{2\mu}{\hbar^2}\left(\langle\Psi_V|\,\hat{V}^c_{\rm rel} - \hat{V}^c_{\mathcal{C}}\,|\mathcal{G}_{V,c}\rangle - \langle\Psi_V|\,\hat{V}^c_{\rm rel} - \frac{\hbar^2}{2\mu}\nabla^2_{\rm rel} - E_{\rm rel}\,|\lambda^c(r_c;\gamma)\Psi^c_{1\otimes 2}\rangle - \langle\widetilde{\mathcal{G}}_{V,c}|\,\hat{H} - E_{\rm rel} + E_{V,\alpha}\,|\Psi_V\rangle\right)$$

$$B_{V,c} \approx \frac{2\mu}{\hbar^2}\left(\langle\mathcal{F}_{V,c}|\,\hat{H} - E_{\rm rel} + E_{V,\alpha}\,|\Psi_V\rangle - \langle\Psi_V|\,\hat{V}^c_{\rm rel} - \hat{V}^c_{\mathcal{C}}\,|\mathcal{F}_{V,c}\rangle\right)$$

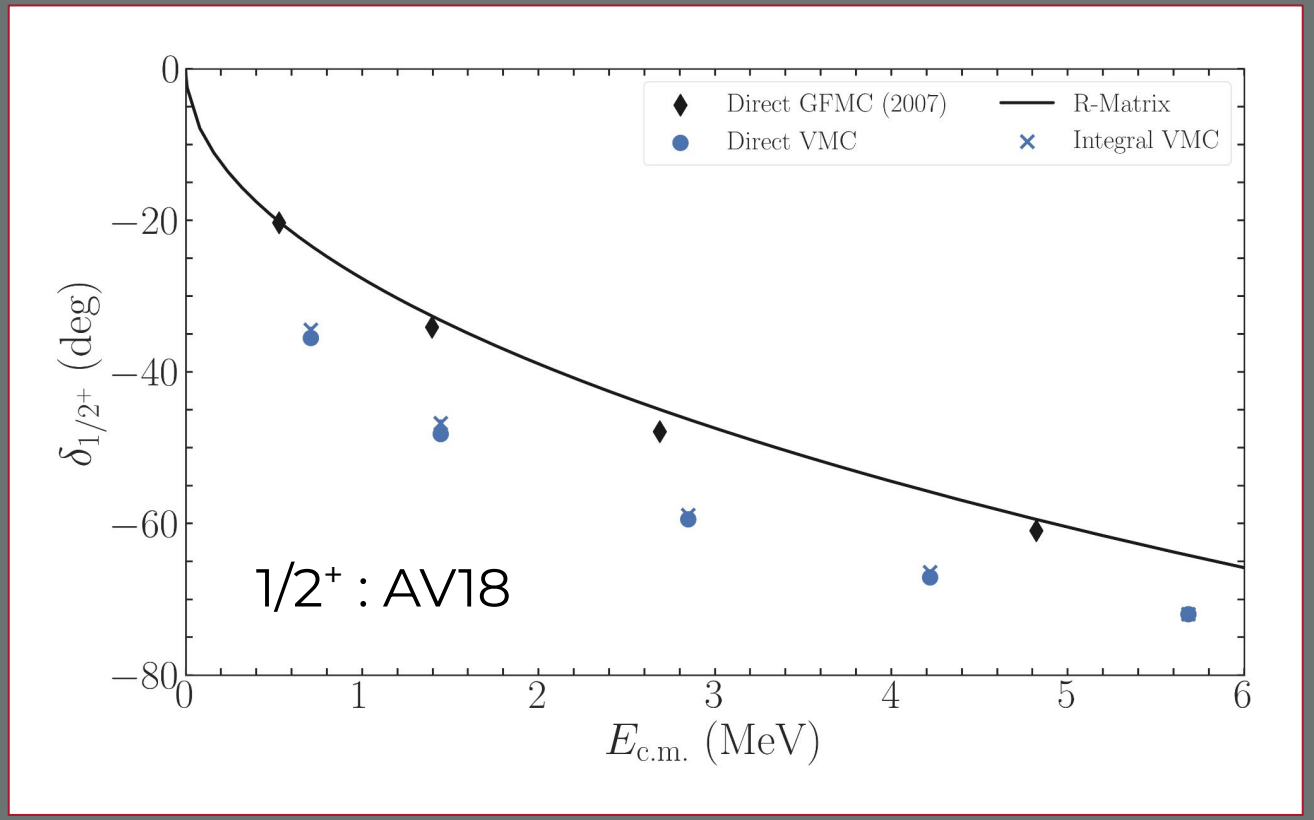
Reasonable assumption for s-shell nuclei (not so reasonable for p-shell VMC)

It is also possible to think of the relative energy as in input parameter for VMC

VMC Phase Shifts

R-matrix from G. Hale (LANL)
GFMC : Nollett *et al* (2007)

n+^{4}He (Single Channel Scattering)



Green's function Monte Carlo (GFMC)

Projecting out the Ground State

$\hbar = 1$
$\tau = it$

The basic concepts of GFMC

$$\lim_{\tau\to\infty} \sum_i e^{-E_i\tau}\alpha_i\Psi_i(\mathbf{R}) = \alpha_{\text{g.s.}}\Psi_{\text{g.s.}}(\mathbf{R})$$

$$\Psi_{\text{g.s.}}(\mathbf{R}) = \lim_{\tau\to\infty} e^{-\hat{H}\tau}\Psi(\mathbf{R},0)$$

The task is then to compute the propagator and the initial wave function

Evolution of the Wave Function

The basic concepts of GFMC

The form of the propagator for arbitrary τ is unreasonable to compute

but... $$e^{-\hat{H}\tau} = \left[e^{-\hat{H}\Delta\tau}\right]^{N_\tau} \qquad N_\tau = \frac{\tau}{\Delta\tau}$$

$$\Delta\tau < 0.001 \text{ MeV}^{-1}$$

The small-time evolution operator can then be written in terms of

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = \langle \mathbf{R}' | \, e^{-\hat{H}\Delta\tau} \, | \mathbf{R} \rangle \qquad |\mathbf{R} - \mathbf{R}'| \sim 0.01 \text{ fm}$$

We can then evolve our wave function in steps of $\Delta\tau$

$$\Psi_{n+1}(\mathbf{R}') = \int G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R}) d\mathbf{R}$$

$$\Psi_n(\mathbf{R}) = \Psi(\mathbf{R}, n\Delta\tau)$$

GFMC Walkers (Monte Carlo Markov Chains)

$$\Psi_{N_\tau}(\mathbf{R}_{N_\tau}) = \int d^{3A}\mathbf{R}_{N_\tau-1} G(\mathbf{R}_{N_\tau}, \mathbf{R}_{N_\tau-1}; \Delta\tau)\Psi_{N_\tau-1}(\mathbf{R}_{N_\tau-1})$$

$$= \int d^{3A}\mathbf{R}_{N_\tau-1} G(\mathbf{R}_{N_\tau}, \mathbf{R}_{N_\tau-1}; \Delta\tau) \int d^{3A}\mathbf{R}_{N_\tau-2} G(\mathbf{R}_{N_\tau-1}, \mathbf{R}_{N_\tau-2}; \Delta\tau) \int d^{3A}\mathbf{R}_{N_\tau-3} G(\mathbf{R}_{N_\tau-2}, \mathbf{R}_{N_\tau-3}; \Delta\tau) \ldots$$

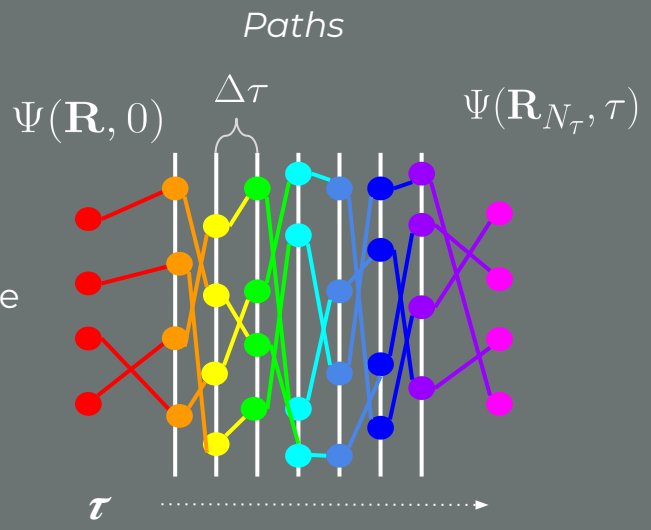
$$\ldots \int d^{3A}\mathbf{R}\, G(\mathbf{R}_1, \mathbf{R}; \Delta\tau)\Psi(\mathbf{R}, 0)$$

We start with many samples of the VMC wave function ($\Psi(\mathbf{R}, 0)$)

Each sample becomes a walker and is propagated in imaginary time

Each walker is then a chain of samples for the integrals above

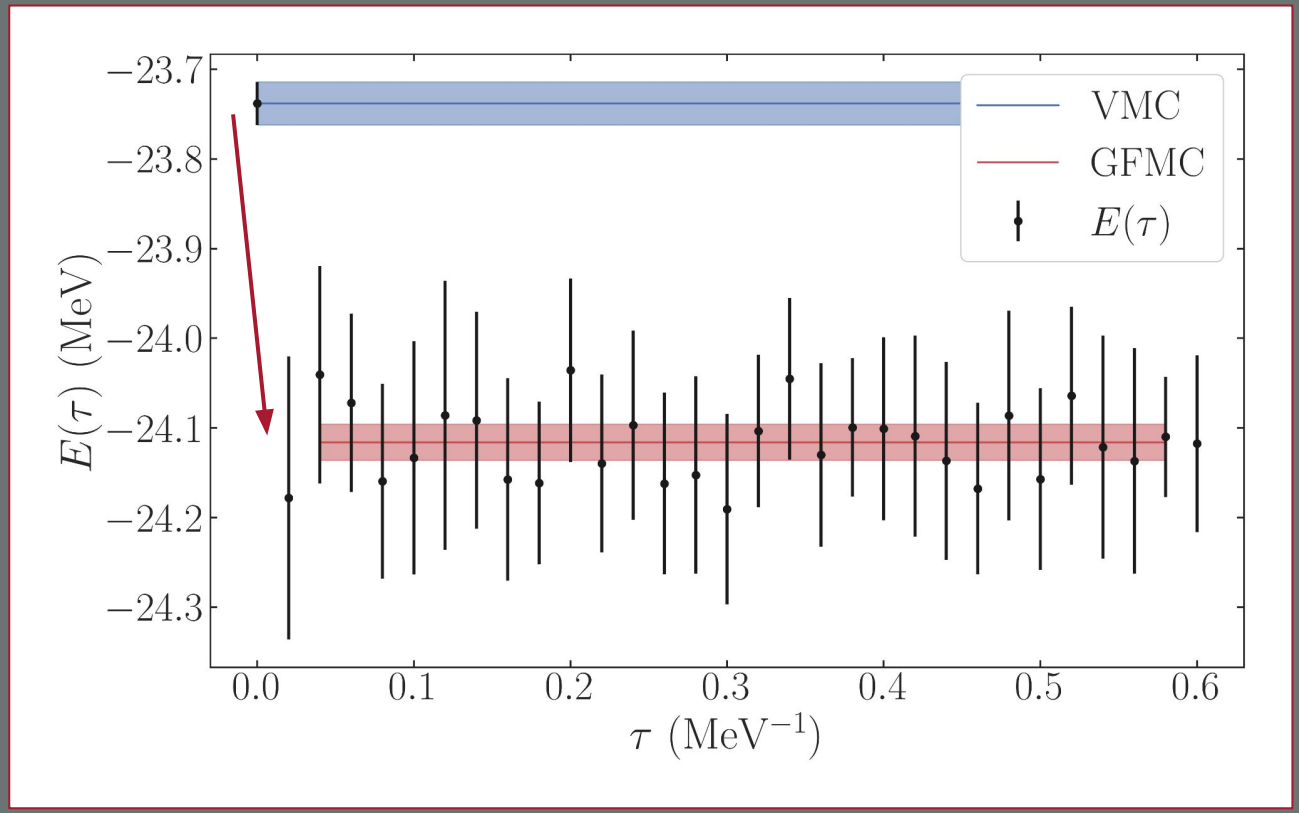
The samples are then used with $\Psi(\mathbf{R}, 0)$ to compute observables



Stabilization of the Energy

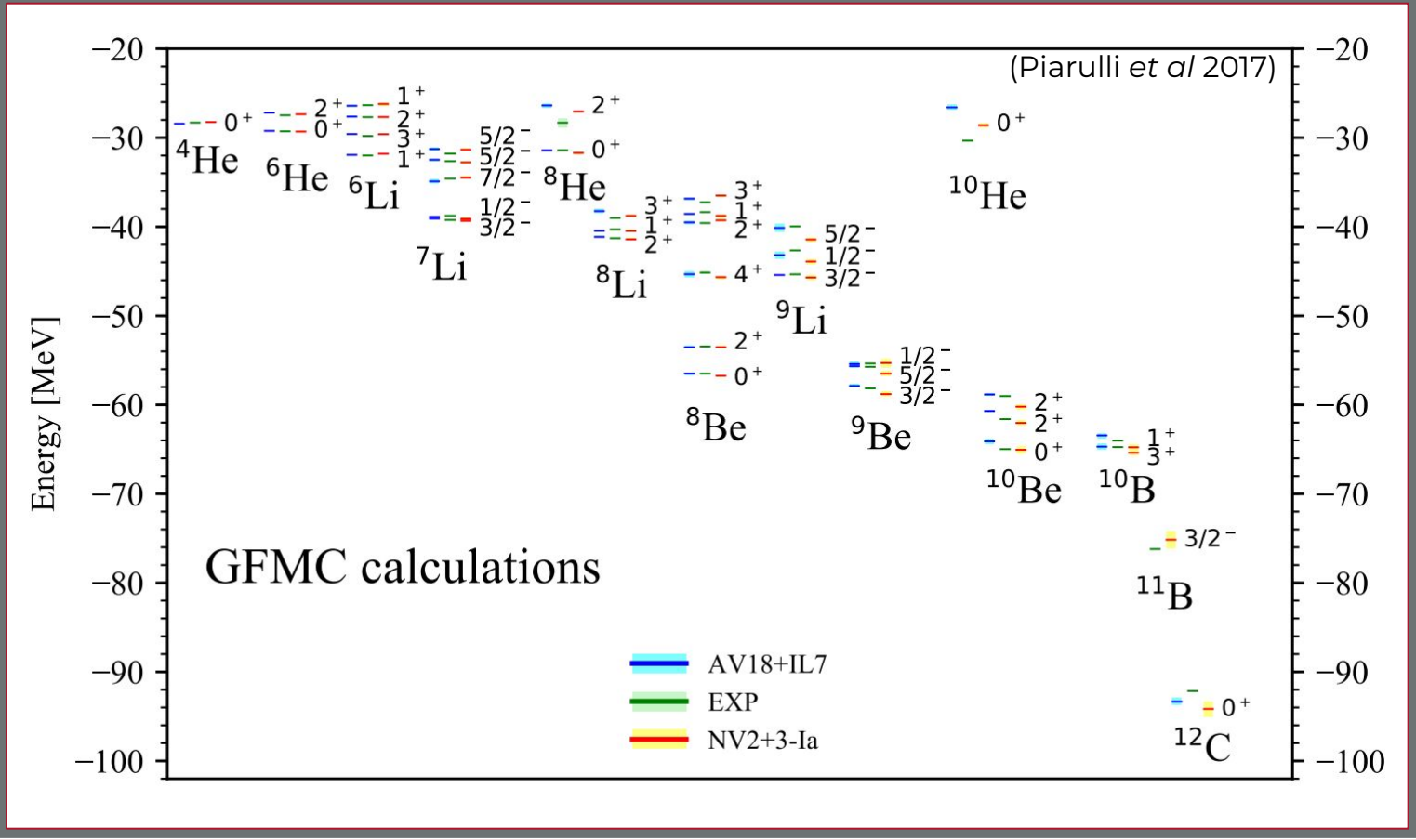
^{4}He : AV18

High energy contamination goes away fast!



Stable samples a used to compute observables

GFMC Energy Spectra (A ≤ 12)



Adapting GFMC to Scattering States

(Nollett *et al* 2007)

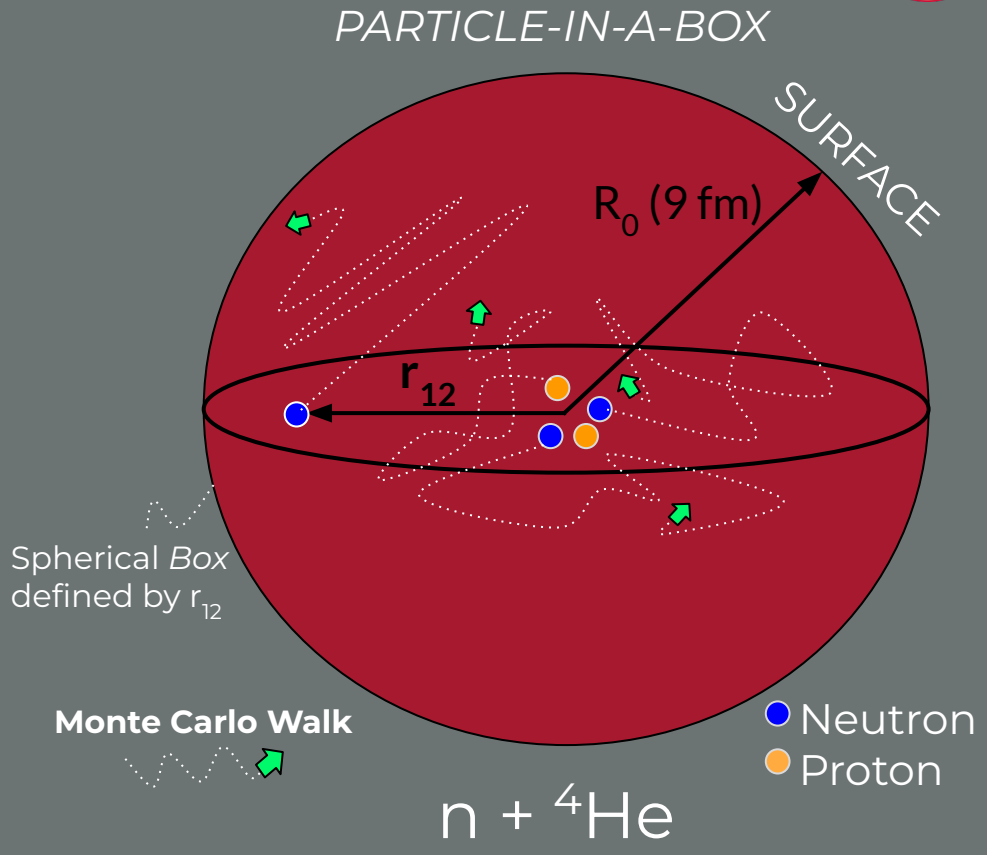
True Scattering Boundary Condition

$$\Psi(\text{all } r_c \to \infty) = \sum_c (A_c \mathcal{F}_c + B_c \mathcal{G}_c)$$

GFMC needs an eigenvalue problem

Log-Derivative Boundary Condition

$$\hat{\mathbf{n}}_c \cdot \nabla_{\mathbf{r}_c} \left(\mathbf{r}_c \left| \Psi \right\rangle \right) = \zeta_c \mathbf{r}_c \left| \Psi \right\rangle$$



Evolving GFMC Scattering States

(Nollett *et al* 2007)

In VMC we were able to insert the boundary condition explicitly

In GFMC we enforce the boundary condition by *method of images* (Carlson)

We can view *particle-in-box* as short-range part of wave function filling all space

$$\Psi_{n+1}(\mathbf{R}') = \underbrace{\int_{|\mathbf{r}_{12}|<R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R})}_{\textit{INSIDE}} + \underbrace{\int_{|\mathbf{r}_{12}|>R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R})}_{\textit{OUTSIDE}}$$

Each walker receives contributions from inside and outside

outside

Method of Images

J. Carlson (Nollett *et al* 2007)

INSIDE *OUTSIDE*

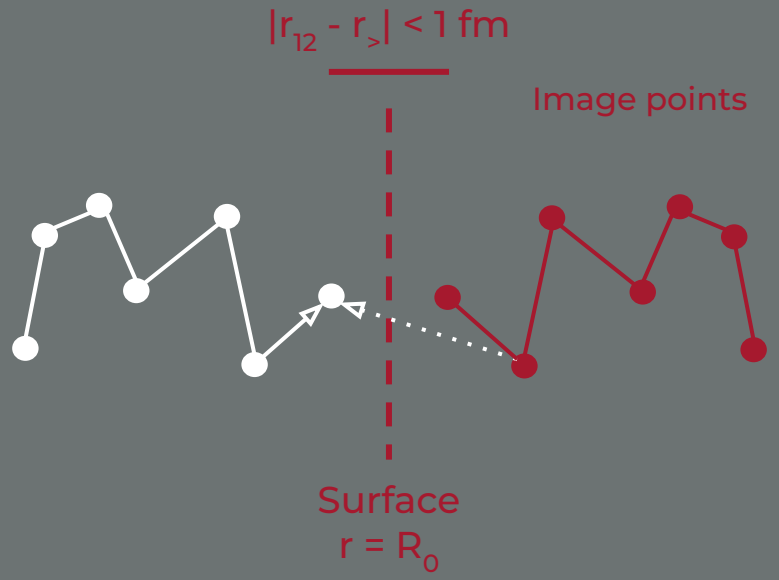
$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_{12}|<R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} \left\{ G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R}) + \left(\frac{r_>}{r}\right)^3 G(\mathbf{R}', \mathbf{R}_>; \Delta\tau)\Psi_n(\mathbf{R}_>) \right\}$$

Map *outside* to *inside* with a change of variables

Use boundary condition to extrapolate to image point

$$\Psi_n(\mathbf{R}_>) \approx \left[1 + \zeta_c(\mathbf{R}_> - \mathbf{R}) \cdot \hat{\mathbf{n}}\right] \Psi_n(\mathbf{R})$$

In practice we only compute image contributions when we are near the surface



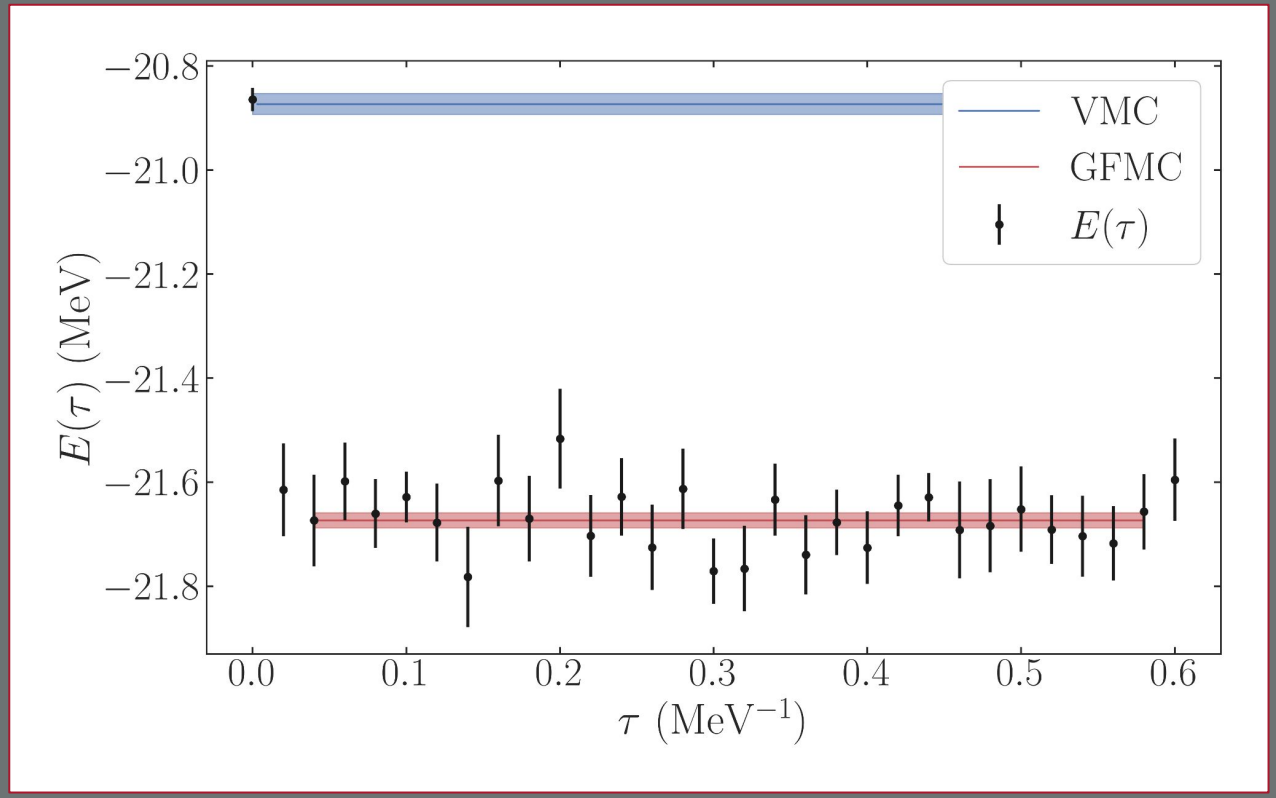
Each inside point has an image point outside

Stabilization of the Energy

^{5}He: 1/2$^+$: AV18

boundary condition (ζ = -0.13 fm^{-1})

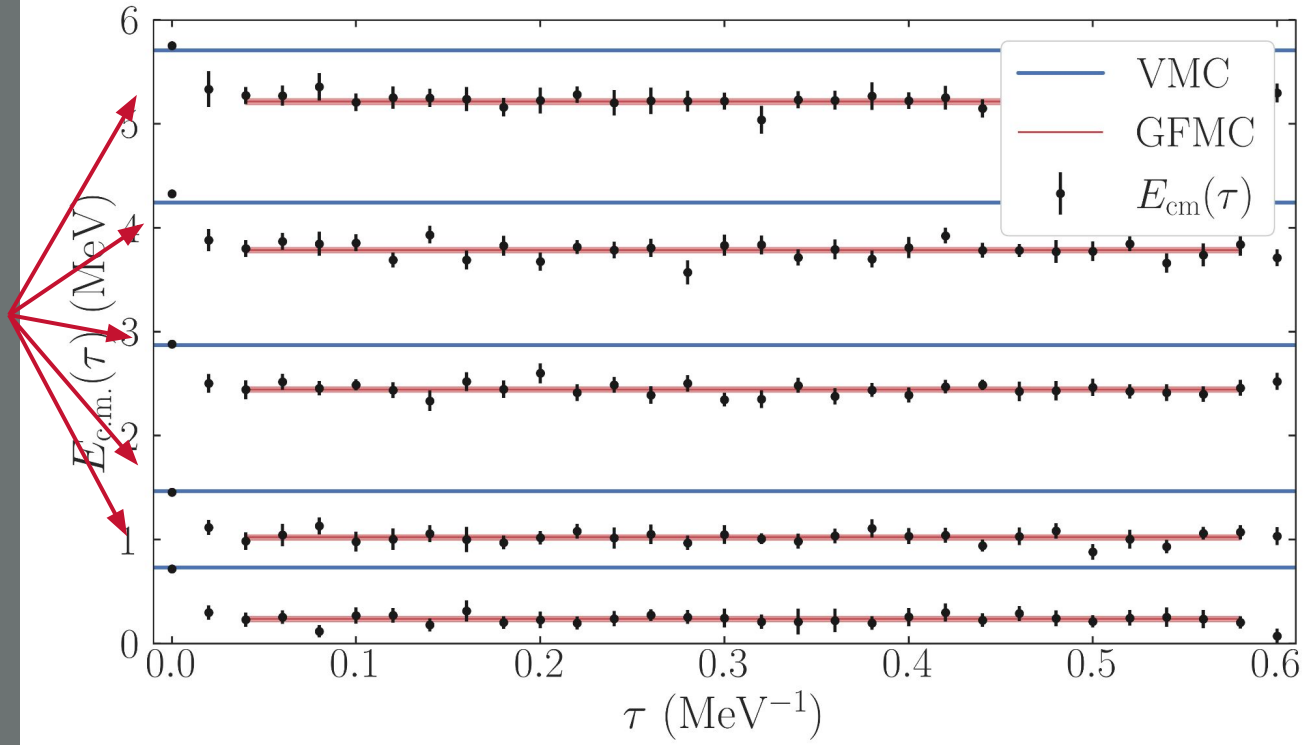
High energy garbage goes away fast



Stabilization of the Energy

^{5}He: 1/2$^+$: AV18

Different boundary conditions ($\boldsymbol{\zeta}$)



Integral Relations with GFMC Wave Functions

Ideally we want to compute

$$A_c(\tau) = \frac{2\mu}{\hbar^2}\left(\langle\Psi(\tau)|\,\hat{H}-E\,|\widetilde{\mathcal{G}}_c(\tau)\rangle - \langle\widetilde{\mathcal{G}}_c(\tau)|\,\hat{H}-E\,|\Psi(\tau)\rangle\right)$$

$$B_c(\tau) = \frac{2\mu}{\hbar^2}\left(\langle\mathcal{F}_c(\tau)|\,\hat{H}-E\,|\Psi(\tau)\rangle - \langle\Psi(\tau)|\,\hat{H}-E\,|\mathcal{F}_c(\tau)\rangle\right)$$

Integral Relations with GFMC Wave Functions

Eigenstate Assumptions

In practice we assume that

$$(\hat{H}_\alpha - E_\alpha)\,|\Psi_\alpha(\tau)\rangle = 0 \qquad \text{and} \qquad (\hat{H} - E)\,|\Psi(\tau)\rangle = 0$$

$$A_c(\tau) \approx \frac{2\mu}{\hbar^2}\,\langle \Psi(\tau)|\,\hat{V}_{\text{rel}} - \hat{V}_{\mathcal{C}}\,|\widetilde{\mathcal{G}}_c(\tau)\rangle$$

$$B_c(\tau) \approx -\frac{2\mu}{\hbar^2}\,\langle \Psi(\tau)|\,\hat{V}_{\text{rel}} - \hat{V}_{\mathcal{C}}\,|\mathcal{F}_c(\tau)\rangle$$

This requires a special kind of mixed estimates
*expansion in (GFMC - VMC)

Single Channel Scattering

match smoothly across the boundary to get

Direct Method

$$\tan\delta = \left.\frac{k\frac{\partial}{\partial\rho}F_l(\eta,\rho) - \zeta F_l(\eta,\rho)}{\zeta G_l(\eta,\rho) - k\frac{\partial}{\partial\rho}G_l(\eta,\rho)}\right|_{\rho=kR_0}$$

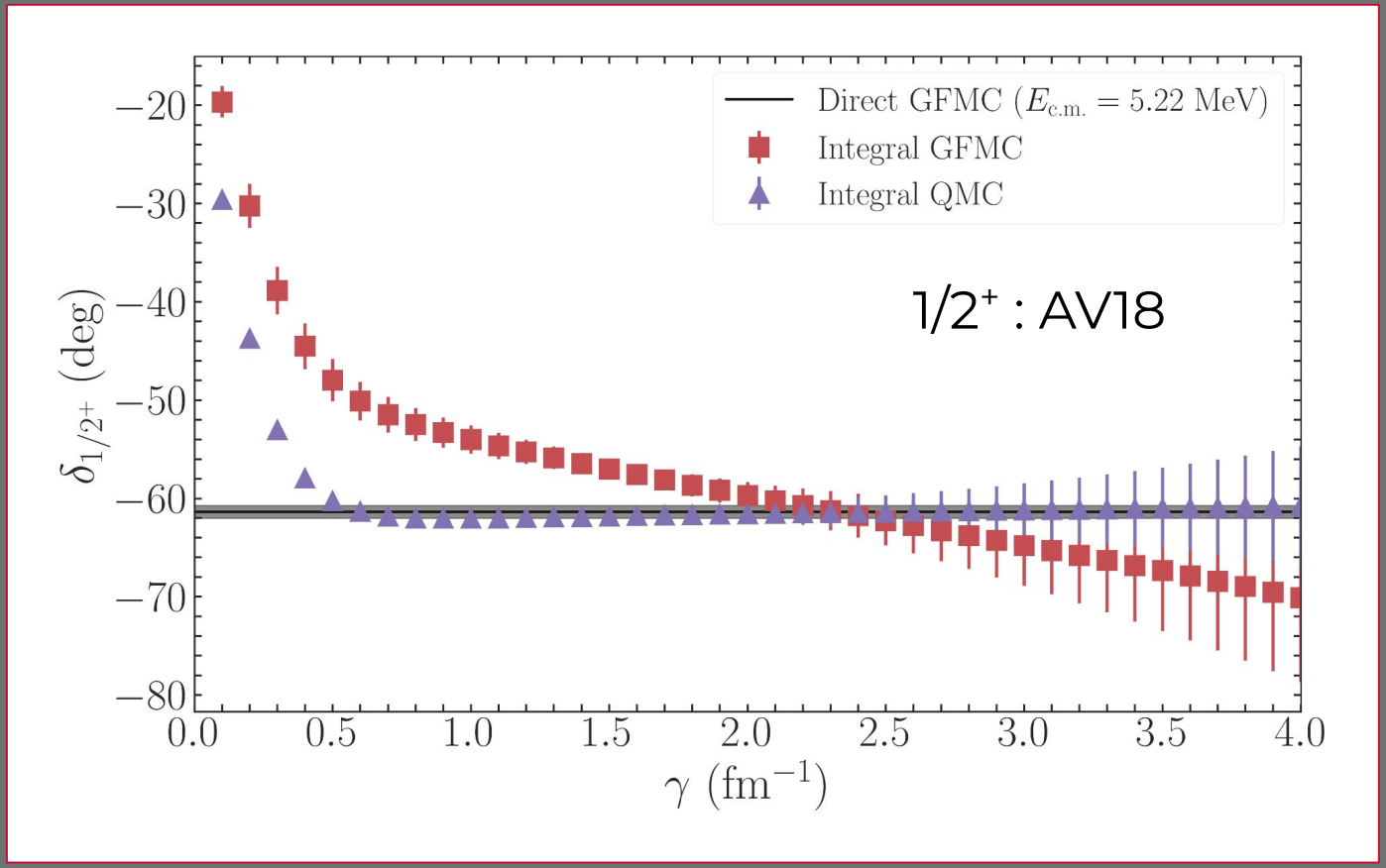
Requires boundary condition + Energy

or

$$\tan\delta = \frac{B}{A}$$

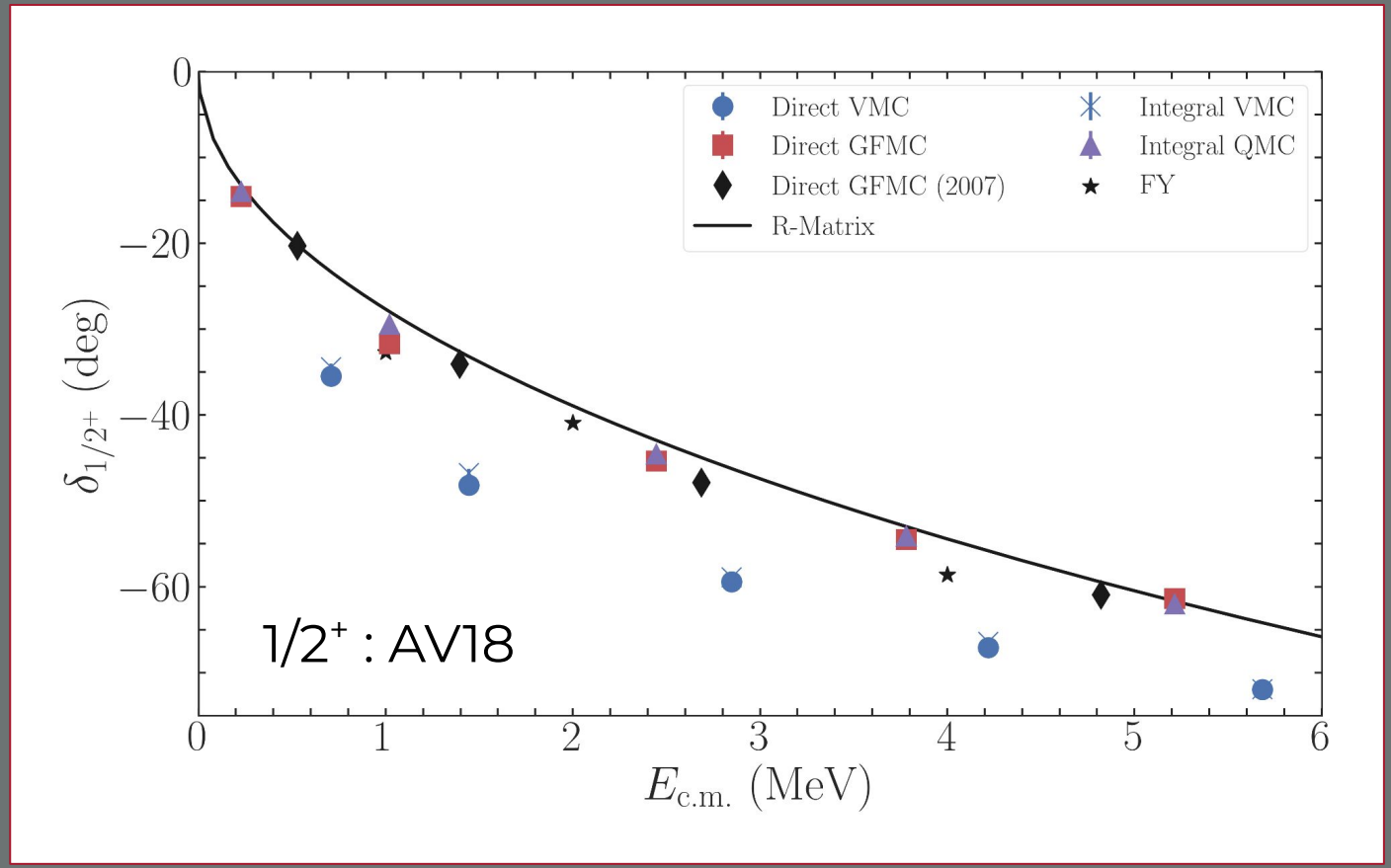
Requires surface amplitudes

Verification of Regularizer



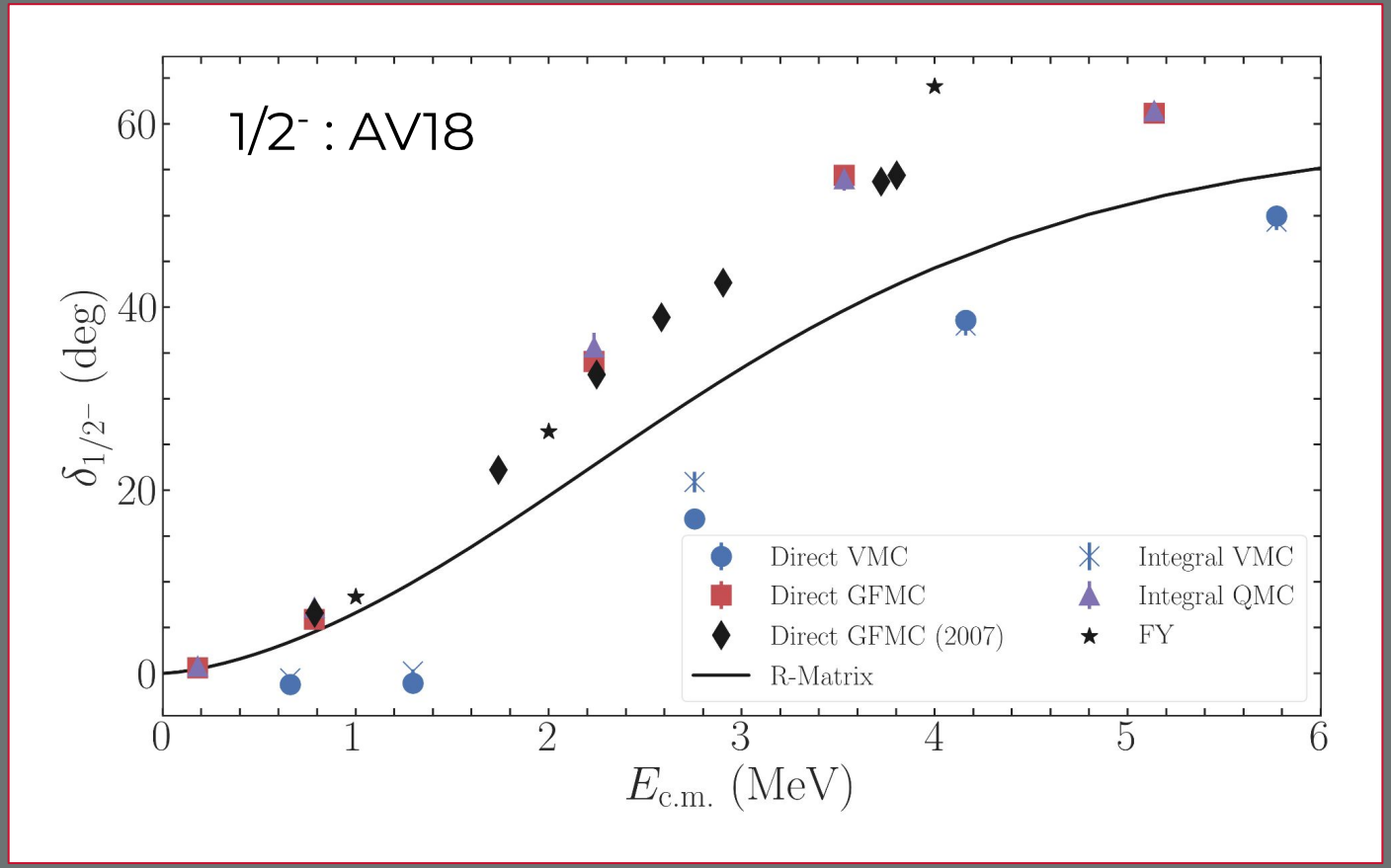
neutron + alpha scattering (n+^{4}He)

R-matrix from (Hale unpublished)
Faddeev-Yakubovsky from (Lazauskas 2018)



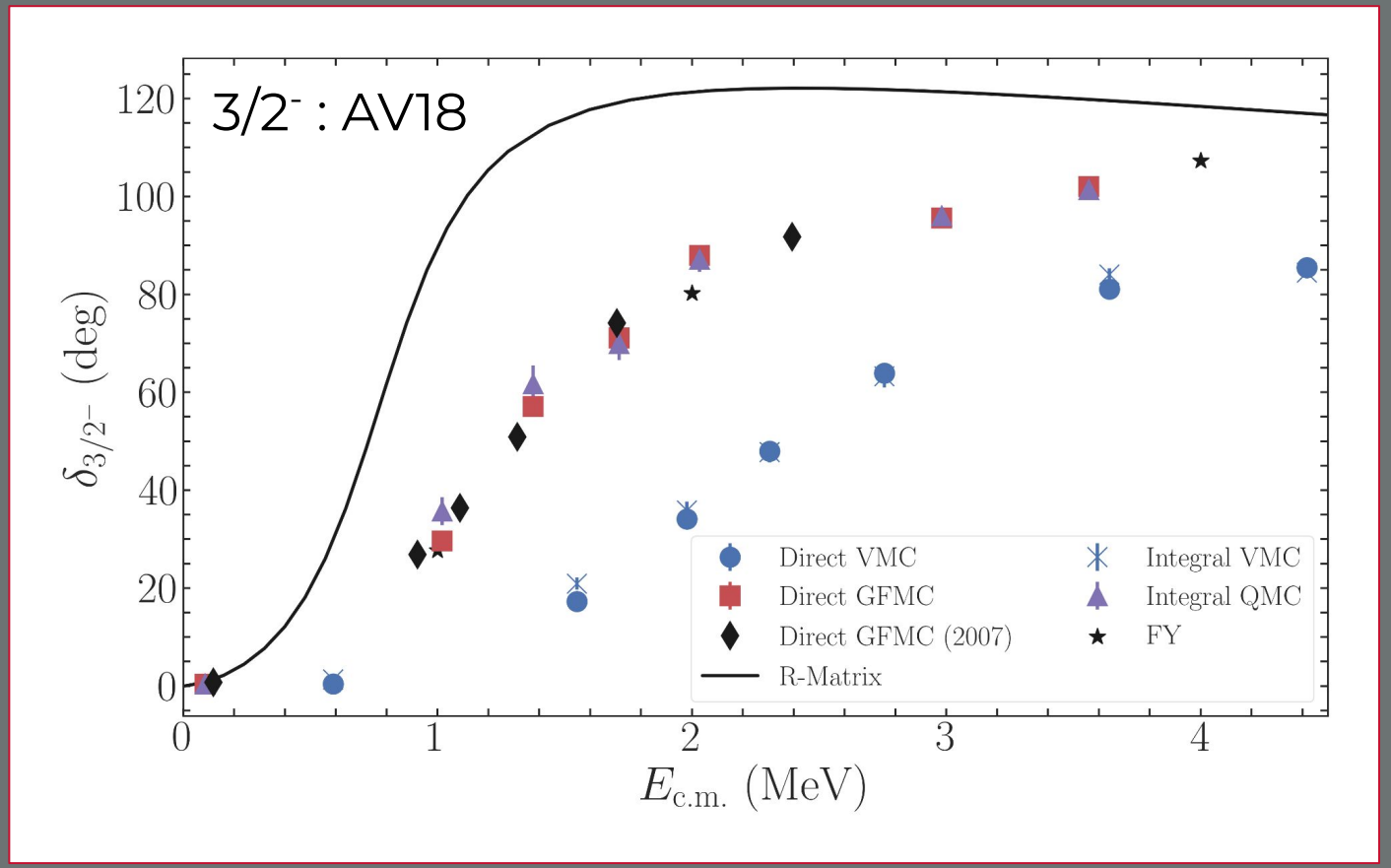
neutron + alpha scattering (n+^{4}He)

R-matrix from (Hale unpublished)
Faddeev-Yakubovsky from (Lazauskas 2018)



neutron + alpha scattering (n+^{4}He)

R-matrix from (Hale unpublished)
Faddeev-Yakubovsky from (Lazauskas 2018)



This Opens the Door to...

- Similar calculations in other light nuclei (extend to p-shell)
- Benchmark and complementarity to other *ab initio* methods (A > 4)
- Unbound T=0 states in ^{4}He (orthogonalization to ground state takes effort)
- Electromagnetic and weak capture reactions (main interest for astrophysics, e.g., $^3\mathrm{He}(\alpha,\gamma)^7\mathrm{Be}$ $^7\mathrm{Be}(p,\gamma)^8\mathrm{B}$)
- Reactions with nuclear rearrangement (e.g., $^3\mathrm{H}(d,n)^4\mathrm{He}$) (after a lot of code development)

All of this means improved data for Norfolk-type interactions

Thanks For Listening!

Work Supported by the US Department of Energy, Office of Nuclear Physics Award DE-SC0019257 (K.M.N)
Work Supported by the 2021 Early Career Award No. DE-SC0022002 and the FRIB Theory Alliance Award No. DE-SC0013617 (M.P.)
Work Supported by DOE DE-SC0021027 (S.P.)

The many-body calculations were performed on the parallel computers of the Laboratory Computing Resource Center, Argonne National Laboratory, and the computers of the Argonne Leadership Computing Facility via the INCITE grant “Ab-initio nuclear structure and nuclear reactions.

Current many-body calculations are performed under the support of National Energy Research Scientific Computing Center (NERSC)

Extra Slides

Green's function Monte Carlo (GFMC)

Time dependent Schrödinger Equation

$$i\frac{\partial}{\partial t}\Psi(\mathbf{R},t) = \hat{H}\Psi(\mathbf{R},t)$$

General Solution

$$\Psi(\mathbf{R},t) = e^{-i\hat{H}t}\Psi(\mathbf{R},0)$$

Schrödinger Equation in Imaginary Time ($\tau = it$)

The basic concepts of GFMC

$$\Psi(\mathbf{R}, \tau) = e^{-\hat{H}\tau}\Psi(\mathbf{R}, 0)$$

The wave function could be represented from the eigenfunctions and eigenvalues of the Hamiltonian

$$\Psi(\mathbf{R}, 0) = \sum_i \alpha_i \Psi_i(\mathbf{R})$$

$$e^{-\hat{H}\tau}\Psi(\mathbf{R}, 0) = \sum_i e^{-E_i\tau}\alpha_i \Psi_i(\mathbf{R})$$

Computing Expectation Values

$$\langle \mathcal{O}(\tau) \rangle = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}$$

We can compute $\Psi(0)$ anywhere

$$\langle \mathcal{O}(\tau) \rangle_{\text{mixed}} = \frac{\langle \Psi(0) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(0) | \Psi(\tau) \rangle}$$

$$\langle \mathcal{O}(\tau) \rangle \approx 2 \langle \mathcal{O}(\tau) \rangle_{\text{mixed}} - \langle \mathcal{O} \rangle_{\text{VMC}}$$

$$E(\tau) = \frac{\langle \Psi(0) | \hat{H} | \Psi(\tau) \rangle}{\langle \Psi(0) | \Psi(\tau) \rangle} = \frac{\langle \Psi(\tau/2) | \hat{H} | \Psi(\tau/2) \rangle}{\langle \Psi(\tau/2) | \Psi(\tau/2) \rangle}$$

Propagate until the energy stabilizes

Many-Nucleon Schrödinger Equation

A = Number of nucleons

$$\hat{H}\,|\Psi(\mathbf{R}, J^\pi, T, T_z)\rangle = E\,|\Psi(\mathbf{R}, J^\pi, T, T_z)\rangle$$

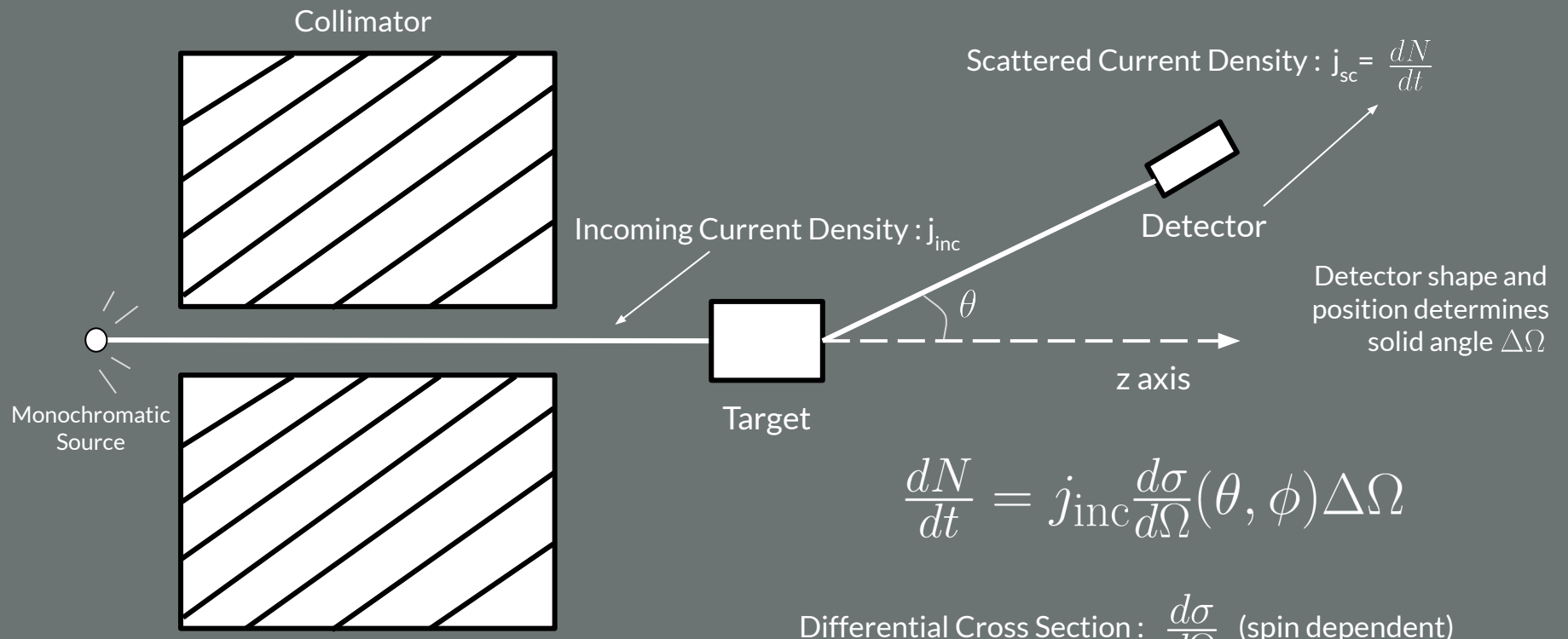
$$\hat{H} = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} V_{ijk}$$

Kinetic Energy + Two-body + Three-body

\+ Scattering Boundary Condition (more on that later)

Experimental Scattering Setup

Depends on Projectile Energy



$$\frac{dN}{dt} = j_{\text{inc}} \frac{d\sigma}{d\Omega}(\theta, \phi)\Delta\Omega$$

Differential Cross Section : $\frac{d\sigma}{d\Omega}$ (spin dependent)

Total Cross Section : integrate over all angles

Rodberg & Thaler (1967). Introduction to the quantum theory of scattering.

Integral Relations with GFMC Wave Functions

Off-diagonal mixed estimates

Ideally ...

$$A_c(\tau) \approx \frac{2\mu}{\hbar^2} \langle \Psi(\tau) | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \widetilde{\mathcal{G}}_c(\tau) \rangle$$

$$B_c(\tau) \approx -\frac{2\mu}{\hbar^2} \langle \Psi(\tau) | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \mathcal{F}_c(\tau) \rangle$$

In practice ...

Propagated Target : ^{4}He

$$A_c(\alpha(\tau)) \equiv \frac{2\mu}{\hbar^2} \langle \widetilde{\mathcal{G}}_c(\tau) | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \Psi_{\rm V} \rangle$$

$$B_c(\alpha(\tau)) \equiv -\frac{2\mu}{\hbar^2} \langle \mathcal{F}_c(\tau) | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \Psi_{\rm V} \rangle$$

Propagated ^{5}He scattering wave function

$$A_c(^5\mathrm{He}(\tau)) \equiv \frac{2\mu}{\hbar^2} \langle \widetilde{\mathcal{G}}_{c,\rm V} | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \Psi(\tau) \rangle$$

$$B_c(^5\mathrm{He}(\tau)) \equiv -\frac{2\mu}{\hbar^2} \langle \mathcal{F}_{c,\rm V} | \hat{V}_{\rm rel} - \hat{V}_{\mathcal{C}} | \Psi(\tau) \rangle$$

Integral Relations with GFMC Wave Functions

Off-diagonal mixed estimates

This requires a special kind of mixed estimates

$$A_c(\tau) \approx \frac{A_c(^5\mathrm{He}(\tau))}{\mathcal{N}_{^5\mathrm{He}(\tau)}} + \frac{A_c(\alpha(\tau))}{\mathcal{N}_{\alpha(\tau)}} - \frac{A_{c,\mathrm{V}}}{\mathcal{N}_V}$$

$$B_c(\tau) \approx \frac{B_c(^5\mathrm{He}(\tau))}{\mathcal{N}_{^5\mathrm{He}(\tau)}} + \frac{B_c(\alpha(\tau))}{\mathcal{N}_{\alpha(\tau)}} - \frac{B_{c,\mathrm{V}}}{\mathcal{N}_V}$$

Neutron Scattering from Tritium (n + ^{3}H)

A Cheap Test Case (problem grows fast with A)

- Small non-trivial case of nuclear scattering that encompses relevent mechanics
- Single and Coupled Channel Scattering
- Available experimental results (Phillips 1980, Hale 1990)
- Computational benchmarks with various potentials and *ab initio* methods (Rev. C 84, 054010 (2011))
    - Alt-Grassberger-Sandhas (Deltuva & Fonseca)
    - Hyperspherical Harmonics (Viviani, Kievsky, Marcucci, Rosati)
    - Faddeev-Yakubovsky (Lazauskas & Carbonell)

Neutron Scattering from Alpha (n + ^{4}He)

Another Cheap Test Case (problem grows really fast with A)

* all n + ^{3}H channels are currently not implemented in GFMC ~ 1 month of crucial time to code, verify, and test.

- Small non-trivial case of nuclear scattering that encompses relevent mechanics
- Only single channel
- Available R-matrix calculations (Hale unpublished)
- Computational benchmarks with AV18 potential
  - Faddeev-Yakubovsky (Lazauskas 2018)
  - Direct GFMC (Nollett 2007)

Spectroscopic Overlaps

Off-diagonal mixed estimates

GFMC Direct Method (Brida 2011)

Left + Right - VMC

$$R_c(r;\tau) \approx \frac{1}{\mathcal{N}_L}\langle \Psi^c_{1\otimes 2}(\tau)| \frac{\delta(r-r_c)}{r_c^2} |\Psi_V\rangle + \frac{1}{\mathcal{N}_R}\langle \Psi^c_{1\otimes 2}(\tau=0)| \frac{\delta(r-r_c)}{r_c^2} |\Psi(\tau)\rangle - R_{c,V}(r)$$

GFMC Integral Method

$$R_c(r;\tau) \approx \frac{1}{r}\left\{\bar{A}_c(r;\tau)F_{l_c}(\eta_c, k_c r) + \bar{B}_c(r;\tau)G_{l_c}(\eta_c, k_c r)\right\}$$

mixed estimates : Left + Right - VMC

$$\bar{A}_c(r) = A_c - \frac{2\mu}{\hbar^2}\int_{r_c>r} \Psi^\dagger (V^c_{\rm rel} - V^c_{\mathcal{C}})\mathcal{G}_c\, d^{3A}R \qquad \bar{B}_c(r) = -\frac{2\mu}{\hbar^2}\int_{r_c<r} \Psi^\dagger (V^c_{\rm rel} - V^c_{\mathcal{C}})\mathcal{F}_c\, d^{3A}R$$

Verification of the Integral Method

Spectroscopic Overlaps

Projection of ^{5}He wave function onto neutron-alpha space

Direct Method (definition)

$$R_c(r) = \frac{1}{\mathcal{N}} \langle \Psi^c_{1\otimes 2} | \frac{\delta(r-r_c)}{r_c^2} | \Psi_V \rangle$$

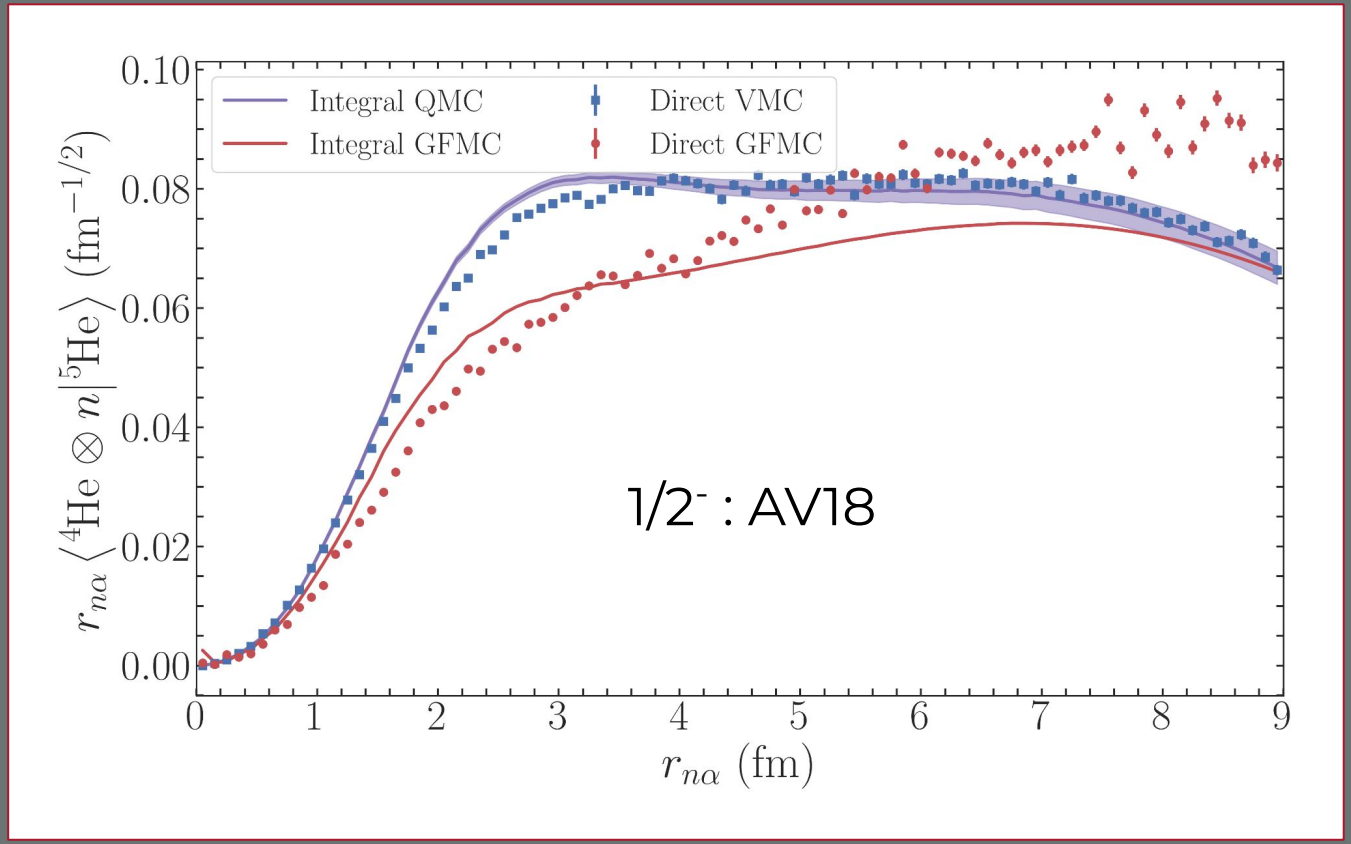
Integral Method

$$R_c(r) = \frac{1}{\mathcal{N} r} \left\{ \bar{A}_c(r) F_{l_c}(\eta_c, k_c r) + \bar{B}_c(r) G_{l_c}(\eta_c, k_c r) \right\}$$

General form of the surface amplitudes at any cluster separation

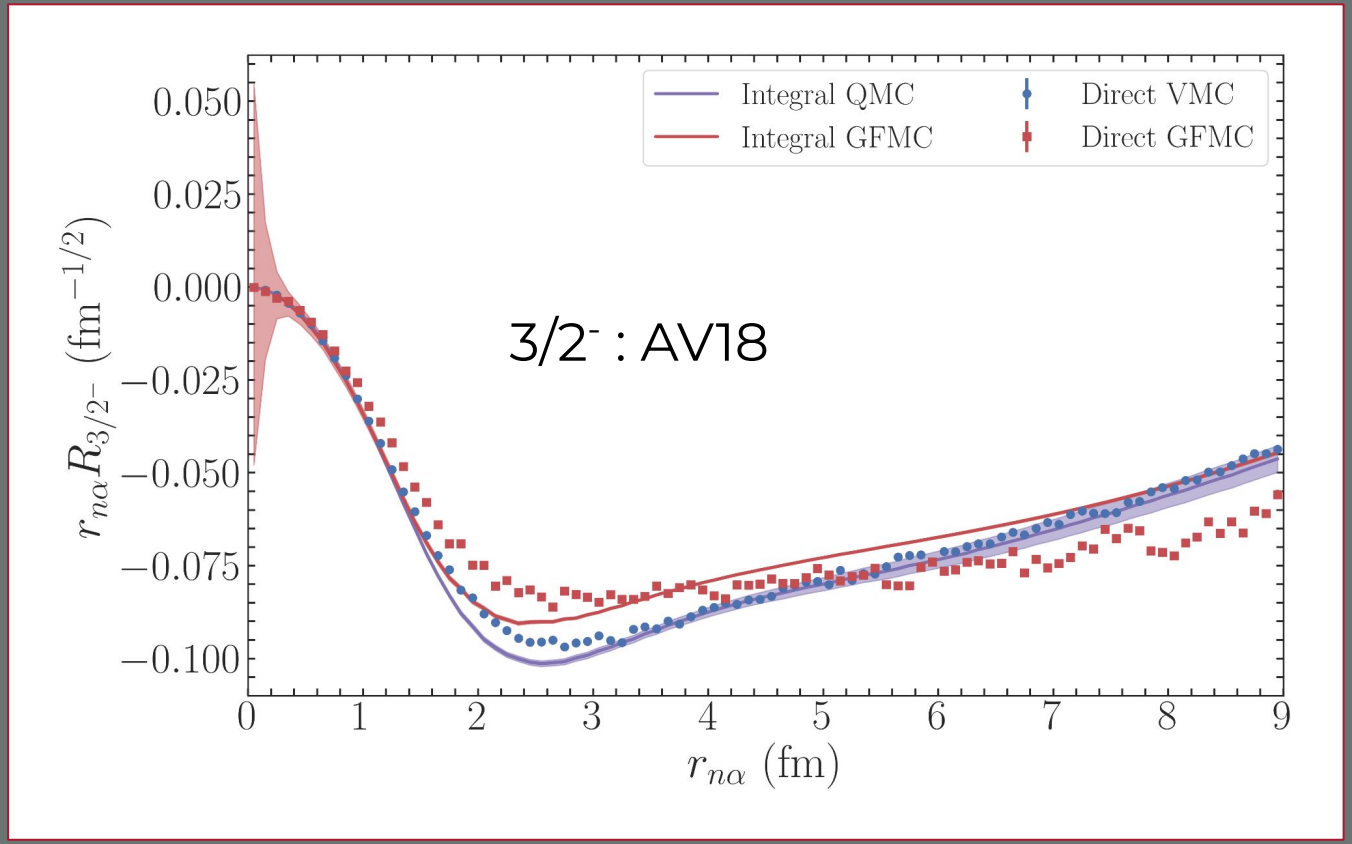
Spectroscopic Overlaps

Off-diagonal mixed estimates



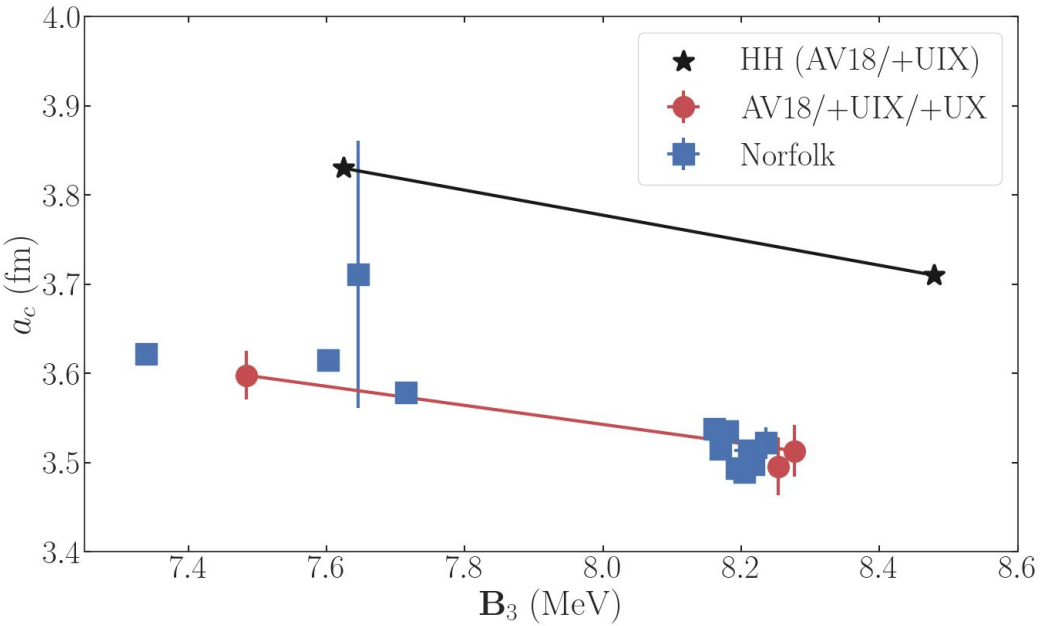
Spectroscopic Overlaps

Off-diagonal mixed estimates



Thermal neutron scattering

Total cross section (barns) , coherent scattering length (fm), and triton binding energy (MeV)



Interaction	σ_t	a_c	B_3
AV18	1.632(12)	3.598(27)	7.484(2)
AV18+UIX	1.558(13)	3.513(29)	8.277(2)
AV18+UX	1.543(15)	3.496(32)	8.254(6)
NVIa	1.648(3)	3.615(6)	7.602(9)
NVIb	1.656(3)	3.622(7)	7.339(9)
NVIIa	1.614(4)	3.579(9)	7.715(5)
NVIIb	1.734(68)	3.711(150)	7.646(14)
NVIa+Ia	1.579(5)	3.535(10)	8.179(9)
NVIb+Ib	1.558(4)	3.515(8)	8.170(15)
NVIIa+IIa	1.539(3)	3.494(6)	8.193(10)
NVIIb+IIb	1.566(8)	3.522(18)	8.236(14)
NVIa+Ia*	1.536(3)	3.490(7)	8.205(8)
NVIb+Ib*	1.580(5)	3.538(11)	8.161(14)
NVIIa+IIa*	1.544(5)	3.498(10)	8.218(17)
NVIIb+IIb*	1.557(5)	3.513(10)	8.212(22)
HH [17, 60]			
AV18	1.85	3.83	7.624
AV18+UIX	1.73	3.71	8.479
R-matrix [85]	-	3.607(17)	-
EXPT.	1.70(3) [88]	3.82(7) [89]	8.475 [91]
		3.59(2) [90]	

(HH from Viviani 2020 and Marcucci 2020) , (R-matrix from Hale 1990), Expt. from (Phillips 1980, Hammerschmied 1981, Rauch 1985, Wang 2012)

Scale of VMC with Nucleons

(Pieper 2001)

	A	Pairs	Spin x Isospin	scale / ^{8}Be	
^{4}H	**4**	**6**	**16 x 4**	**0.002**	
^{5}He	**5**	**10**	**32 x 5**	**0.010**	← **Single Processor**
^{6}Li	6	13	64 x 5	0.036	
^{7}Li	7	21	128 x 14	0.33	
^{8}Be	8	28	256 x 14	1.0	
^{9}Be	9	36	512 x 42	8.7	
^{10}Be	10	43	1024 x 90	52.	
^{11}B	11	55	2048 x 132	200.	
^{12}C	12	66	4096 x 132	530.	← **Supercomputer**

Scale = A*Pairs*Spin*Isospin

*Isospin component has reduced impact.

Adapting VMC to Scattering States

(Carlson 84,87), (Nollett 07), (Lynn 15)

Log-Derivative Boundary Condition

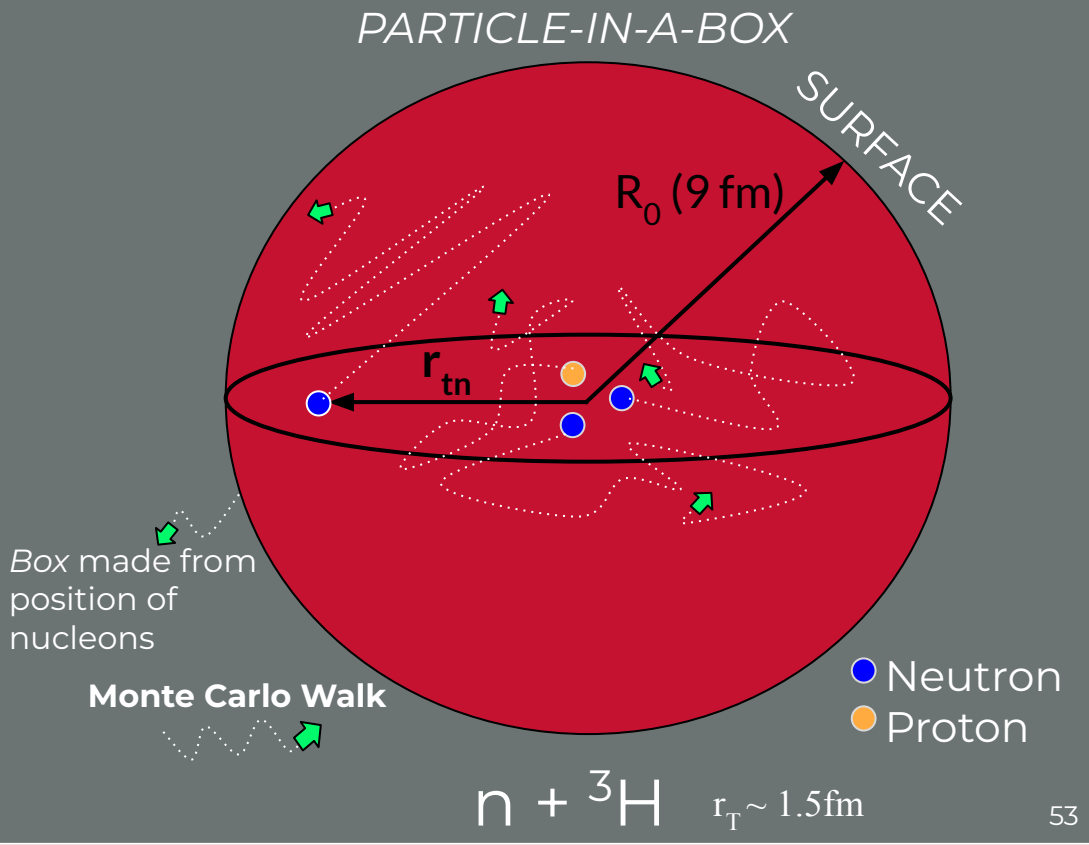
$$\zeta_c u_c(R_0) = \left.\frac{du_c}{dr_c}\right|_{r_c=R_0}$$

$$u_c = r_c \phi_p^{LS[n]} [f_{sp}(r_c)]^{n_{sp}}$$

Scattered nucleon (uses p-shell single particle radial wave function)

boundary condition constant

Minimize E_v in the same way as before



Scattering Formalism

Coulomb wave functions

$$-\frac{d^2u_l}{d\rho^2}+\left(\frac{l(l+1)}{\rho^2}+\frac{2\eta}{\rho}\right)u_l=u_l$$

$$k_c^2=\frac{2\mu E_c}{\hbar^2}$$

$$\rho=k_c r_c$$

$$\eta=\frac{Z_1 Z_2 e^2 \mu}{\hbar^2 k_c}$$

Regular Solution : $F_l(\eta,\rho)$ Irregular Solution : $G_l(\eta,\rho)$

$\eta = 0 \longrightarrow$ spherical Bessel & Neumann functions

Coulomb wave functions describe the asymptotic behavior of the wave function

What is a Channel?

For n + ^{3}H the terms of the partial-wave expansion make up our channels : $^{2S+1}L_J$

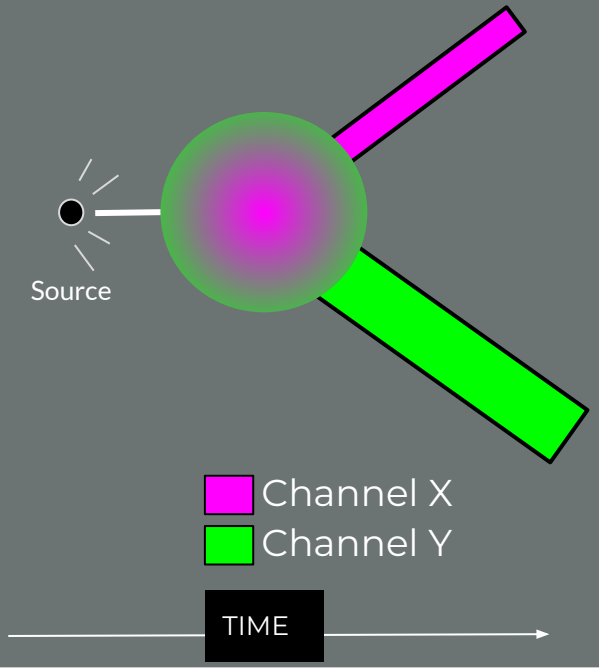
For coupled channel problems S or L can be changed but total angular momentum (J) is conserved.

In nuclear reaction, each possible combination of the target and the source is called a **partition**.

Each partition further distinguished by state of excitation of each nucleus and each such pair of states is known as a reaction **channel**.

In a particular reaction, if **not enough energy** for a particular exit channel then it is said to be **closed**

- Ian Thompson (2009), Nuclear Reactions for Astrophysics



Scattering Formalism

channel-cluster functions

$$\mathcal{F}_c = \Psi^c_{1\otimes 2} \frac{F_{l_c}(\eta_c, k_c r_c)}{k_c r_c} \qquad \mathcal{G}_c = \Psi^c_{1\otimes 2} \frac{G_{l_c}(\eta_c, k_c r_c)}{k_c r_c}$$

$$\Psi^c_{1\otimes 2} = \mathcal{A}_c \left[\psi^{J_{1c}}_{1c} \otimes \left[\psi^{J_{2c}}_{2c} \otimes Y_{l_c}(\hat{r}_c) \right]_{j_c} \right]_J$$

^{3}H or ^{4}He

n

Neutron - Proton Mass Difference

$$K_i = \frac{-\hbar^2}{4}[(\frac{1}{m_p} + \frac{1}{m_n}) + (\frac{1}{m_p} - \frac{1}{m_n})\tau_{iz}]\nabla_i^2$$

Propagator Approximations

The basic concepts of GFMC

$$e^{-\hat{H}\Delta\tau} = e^{-(\hat{T}+\hat{V})\Delta\tau}$$

$$e^{-(\hat{T}+\hat{V})\Delta\tau} \approx e^{-\hat{V}\Delta\tau/2} e^{-\hat{T}\Delta\tau} e^{-\hat{V}\Delta\tau/2} + \mathcal{O}(\Delta\tau^3)$$

Fixed Interior Wave Interpolation (FIWI)

- FIW for two wave functions at the mid-point of their energies
- Average K-matrix (B/A)

$$K_{\mathrm{mid}} = (K_1(E_{\mathrm{mid}}) + K_2(E_{\mathrm{mid}}))/2$$

Should yield a more physically correct curve than FIW alone

Coupled Channel Scattering

The S-matrix (Blatt, Biedenharn 1952)

$$\hat{S} = \hat{O}^T \begin{pmatrix} e^{2i\delta_-} & 0 \\ 0 & e^{2i\delta_+} \end{pmatrix} \hat{O}$$

δ_i : Phase Shift for channel i (coupling scheme independent)

$$\hat{O} = \begin{pmatrix} \cos\epsilon^{J\pi} & \sin\epsilon^{J\pi} \\ -\sin\epsilon^{J\pi} & \cos\epsilon^{J\pi} \end{pmatrix}$$

ϵ : Mixing Parameter (coupling scheme dependent)

For two channel scattering computing the S-matrix requires two linearly independent wave functions at the same energy

The Scattering Matrix

Computing scattering observables

$$m' = \mu -$$

T-matrix

$$M^{ss'}_{\mu\mu'}(\theta) = \frac{\sqrt{4\pi}}{k}\sum_{J=0}^{\infty}\sum_{ll'}\sqrt{2l+1}(l0s\mu|J\mu)(lm's'\mu'|J\mu)T^{ss'}_{ll'}Y_{l'm'}(\theta,0)$$

$$\mathbf{M} = \begin{bmatrix} M^{00} & M^{01} \\ M^{10} & \begin{bmatrix} - & - & - \\ - & M^{11} & - \\ - & - & - \end{bmatrix} \end{bmatrix}$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{4}tr\left\{\mathbf{M}\mathbf{M}^{\dagger}\right\}$$

$$P(\theta) = tr\left\{\mathbf{M}\mathbf{M}^{\dagger}\mathbf{P}\right\}$$

(Kievsky ICTP-SAIFR 2021)

Optimal Parameters for VMC

Constrained Optimization by Linear Approximation (COBYLA)

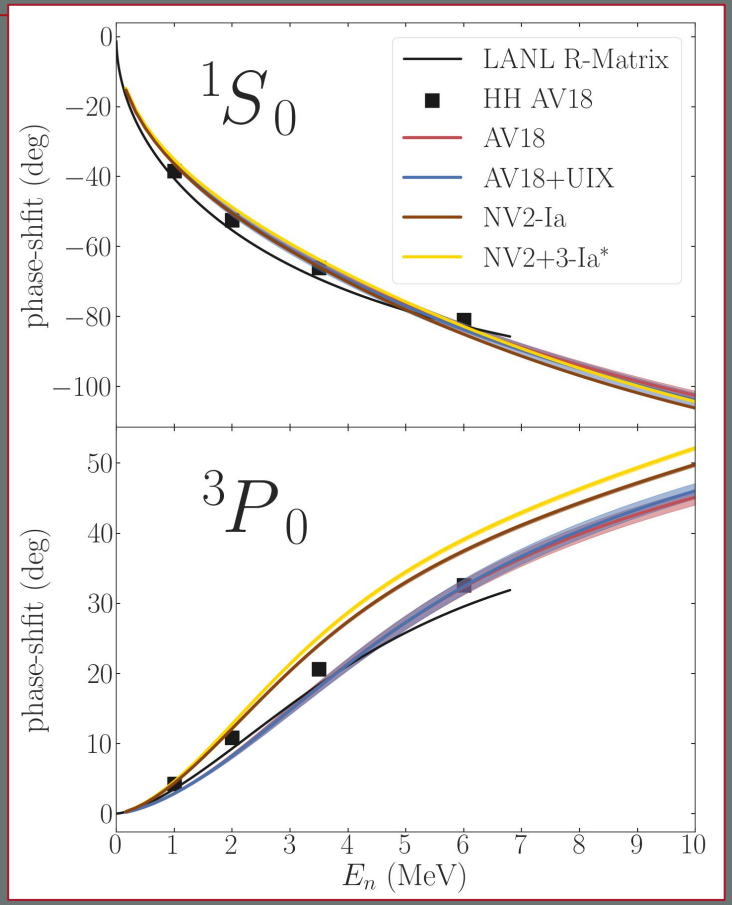
- An iterative algorithm is proposed for nonlinearly constrained optimization calculations when there are no derivatives. Each iteration forms linear approximations to the objective and constraint functions by interpolation at the vertices of a simplex and a trust region bound restricts each change to the variables.
  - M. J. D. Powell. A direct search optimization method that models the objective and constraint functions by linear interpolation. Advances in Optimization and Numerical Analysis, pages 51– 67, 1994.

- Library of Choice
  - NLopt

Single Channel Phase Shifts

Applying the FIW approximation with other interactions.

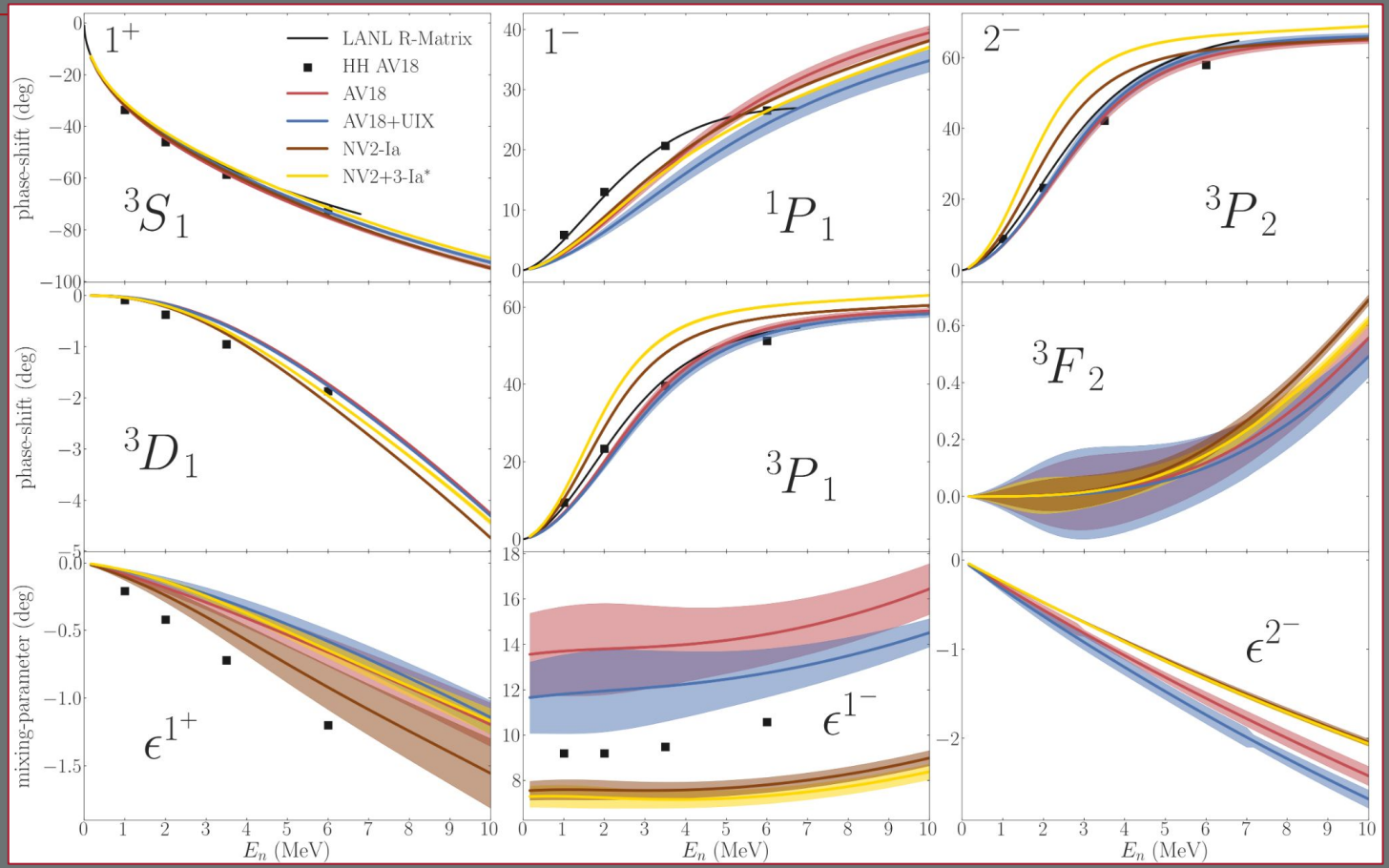
Norfolk models reproduce s-wave scattering but predict a stronger attraction in the p-wave than expected regardless of three-body potential.



LANL R-matrix from (Hale 1990)
Hyperspherical Harmonic method from (Viviani 2011)

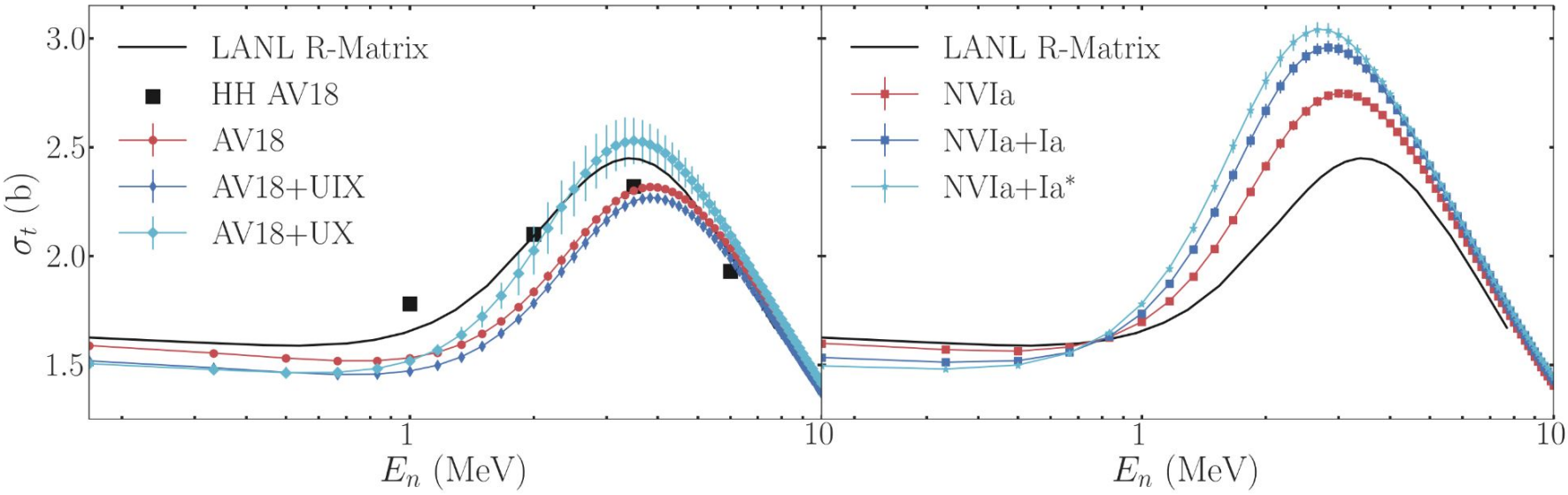
n + ^{3}H Coupled Channel Phase Shifts

VMC Applied successfully to n + ^{3}H scattering



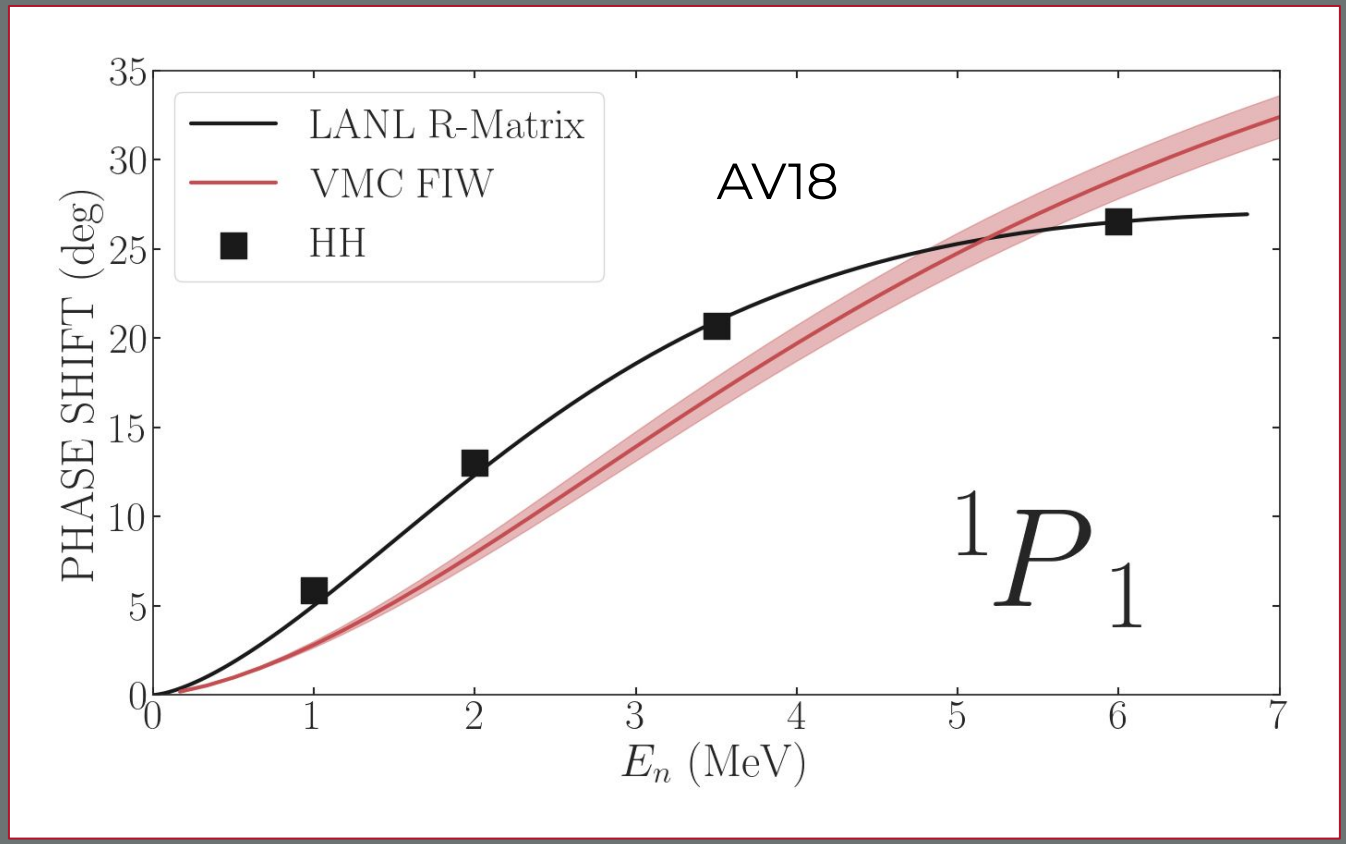
Total Cross Section

LANL R-matrix from (Hale 1990)
Hyperspherical Harmonic method from (Vivia[illegible] 20[illegible])



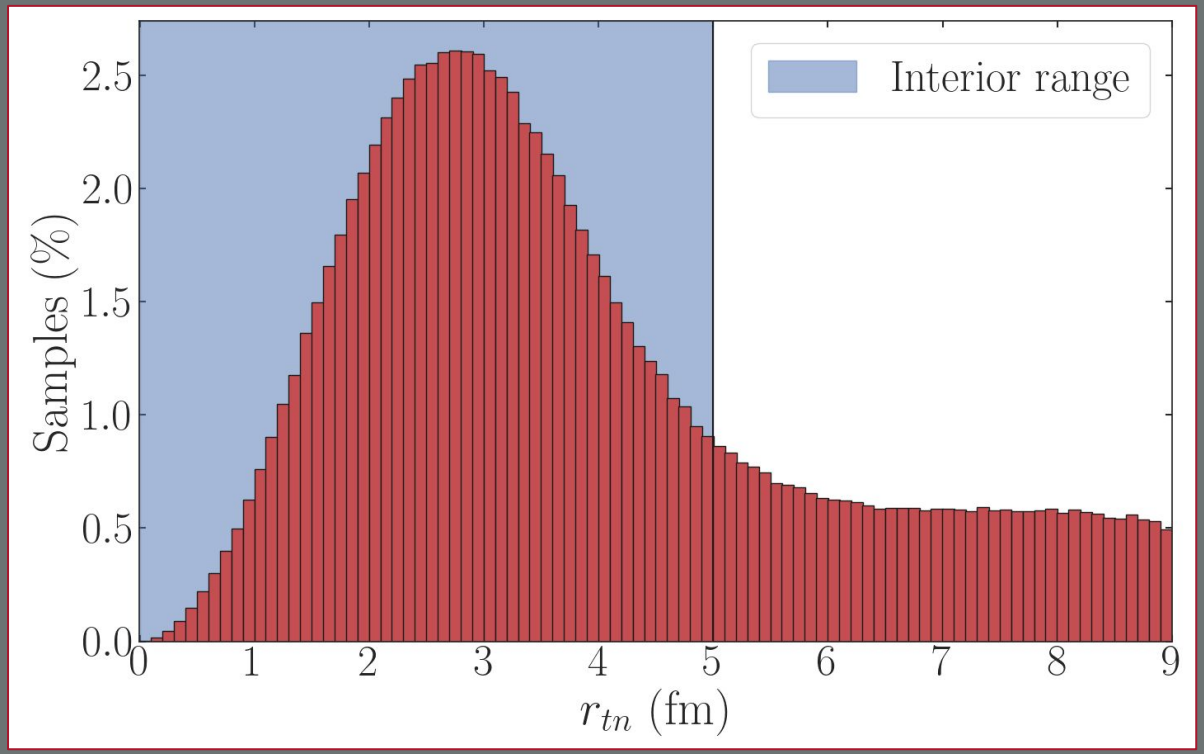
AV18 and AV18+UIX underpredict the strength and width of the resonance feature. All Norfolk interactions (including ones not shown) overpredict the same features.

Singlet 1^- Discrepancy

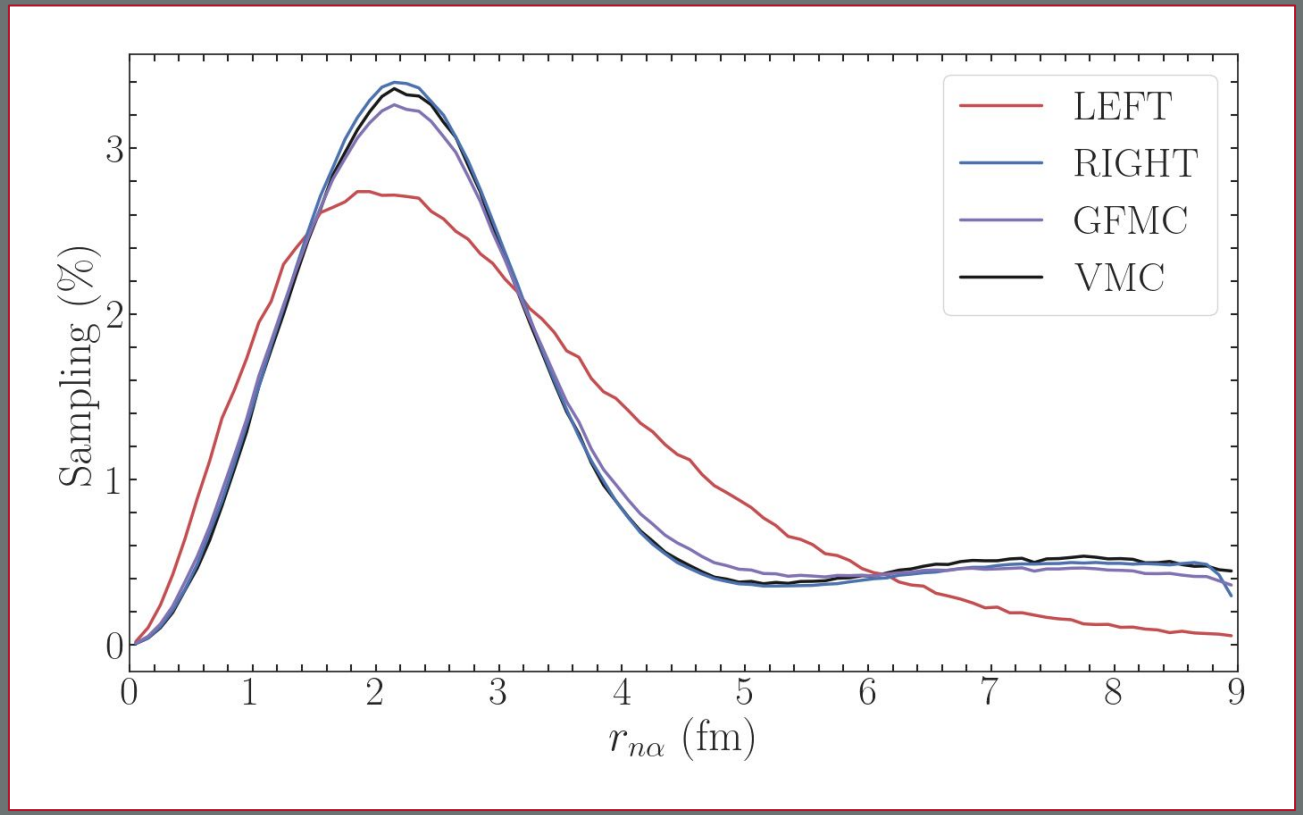


(Hale 1990)
(Viviani 2011)

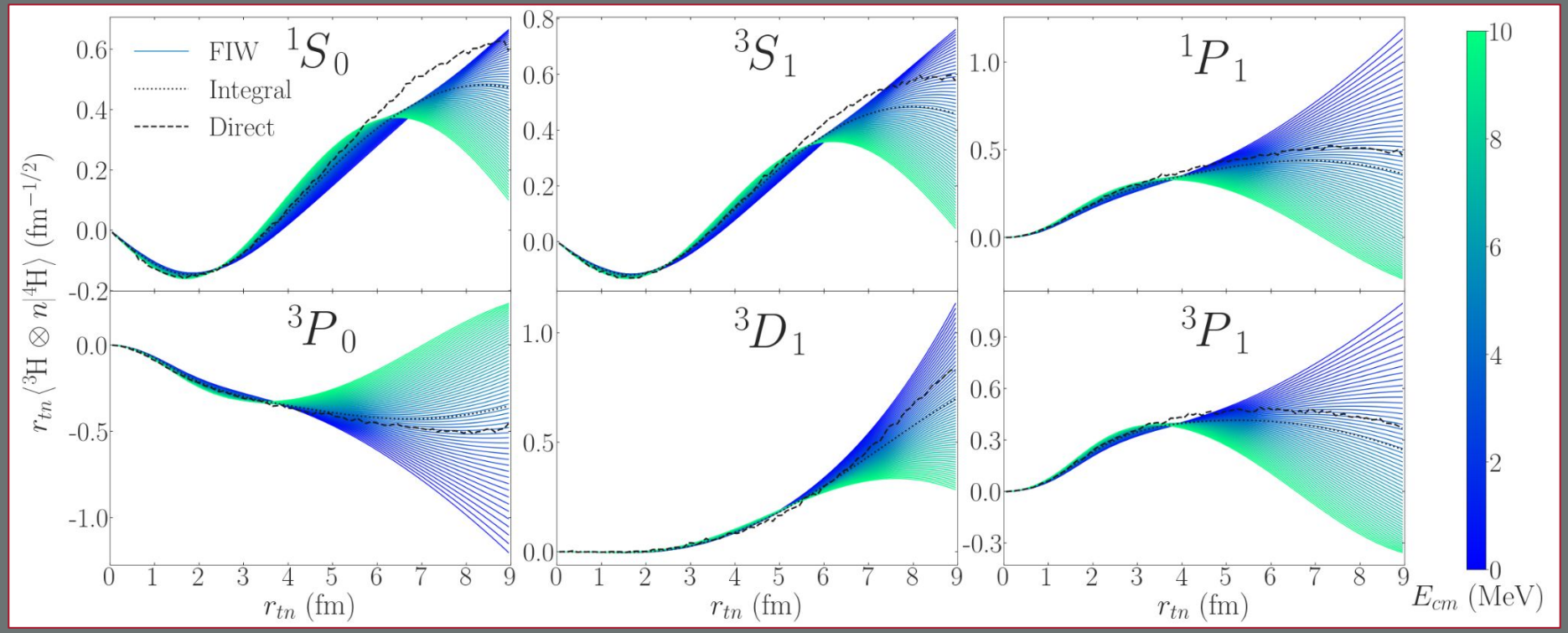
VMC Sampling Bins



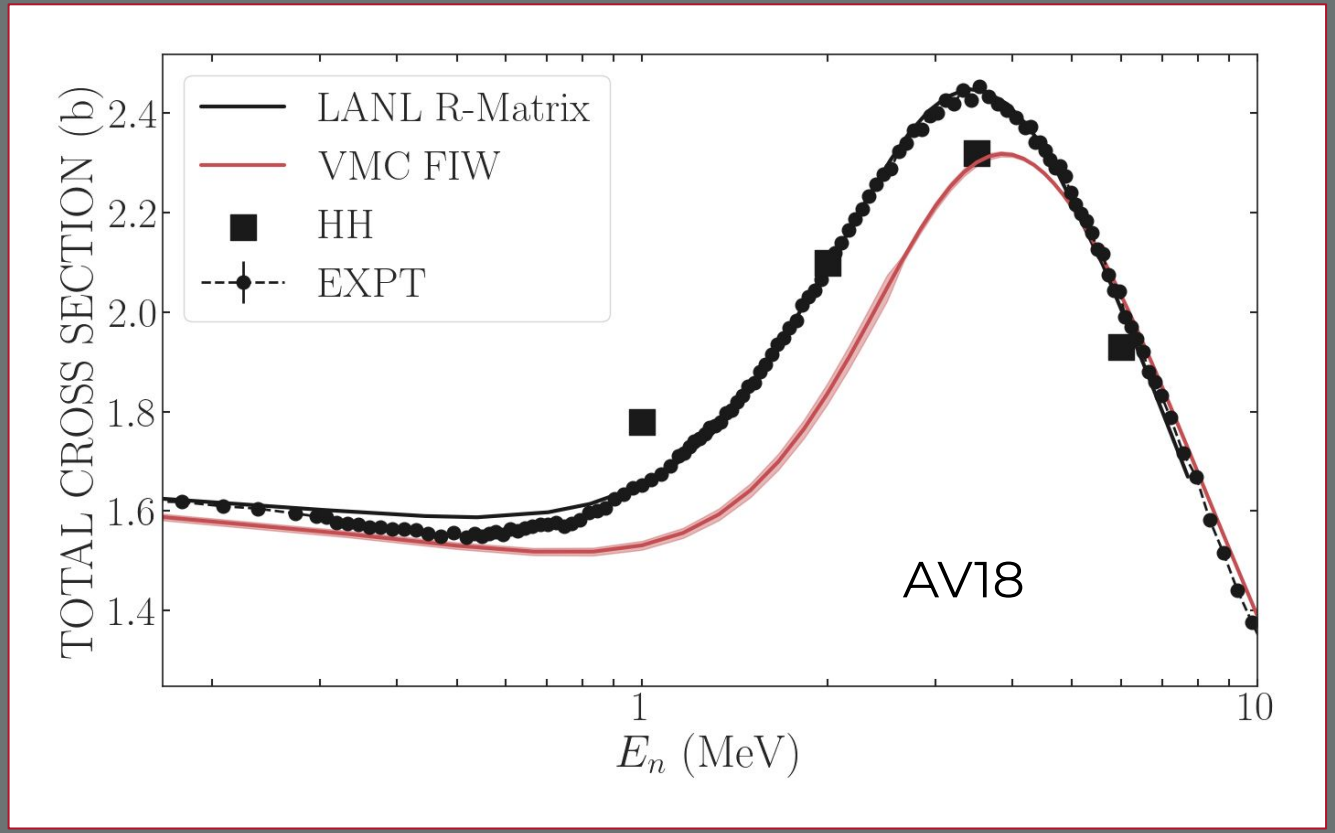
GFMC Sampling Bins



AV18 Overlaps



Total Cross Section



(Philips 1980)
(Hale 1990)
(Viviani 2011)

VMC (n + ^{3}H) Summary

Applied the integral relations to calculations of phase shifts and scattering observables in a variational Monte Carlo context

Developed a validation procedure for the integral relations and regularizer in VMC

Implemented a successful regualizer for the integral relations in VMC

Demonstrated that the Integral relations are a clear improvement over previous QMC methods for unbound systems

Presented the first four-body elastic scattering calculations with the Norfolk interactions

Propagator Approximations (cont.)

The basic concepts of GFMC

The small-time evolution operator can then be written as

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = \langle \mathbf{R}' | \, e^{-\hat{V}\Delta\tau/2} e^{-\hat{T}\Delta\tau} e^{-\hat{V}\Delta\tau/2} \, | \mathbf{R} \rangle$$

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = e^{-\hat{V}\Delta\tau/2} \, \langle \mathbf{R}' | \, e^{-\hat{T}\Delta\tau} \, | \mathbf{R} \rangle \, e^{-\hat{V}\Delta\tau/2}$$

Free Particle Propagator

The basic concepts of GFMC

$$G_o(\mathbf{R}', \mathbf{R}; \Delta\tau) = \langle \mathbf{R}' | \, e^{-\hat{T}\Delta\tau} \, | \mathbf{R} \rangle$$

$$G_o(\mathbf{R}', \mathbf{R}; \Delta\tau) = \left[\frac{m}{32\pi\hbar^2\Delta\tau} \right]^{\frac{3A}{2}} \mathrm{EXP} \left[\frac{-(\mathbf{R} - \mathbf{R}')^2}{\frac{2\hbar^2}{m}\Delta\tau} \right]$$

Importance Sampling

The basic concepts of GFMC

(Pudliner *et al* 19

A new configuration is proposed

$$\mathbf{R}' = \mathbf{R} \pm \delta\mathbf{R}$$

$$W = \left| \sum_{s,t} \langle \Psi_0 | \chi_s \chi_t \rangle \langle \chi_s \chi_t | \Psi(\tau) \rangle \right| + \epsilon \sum_{s,t} |\langle \Psi_0 | \chi_s \chi_t \rangle \langle \chi_s \chi_t | \Psi(\tau) \rangle|$$

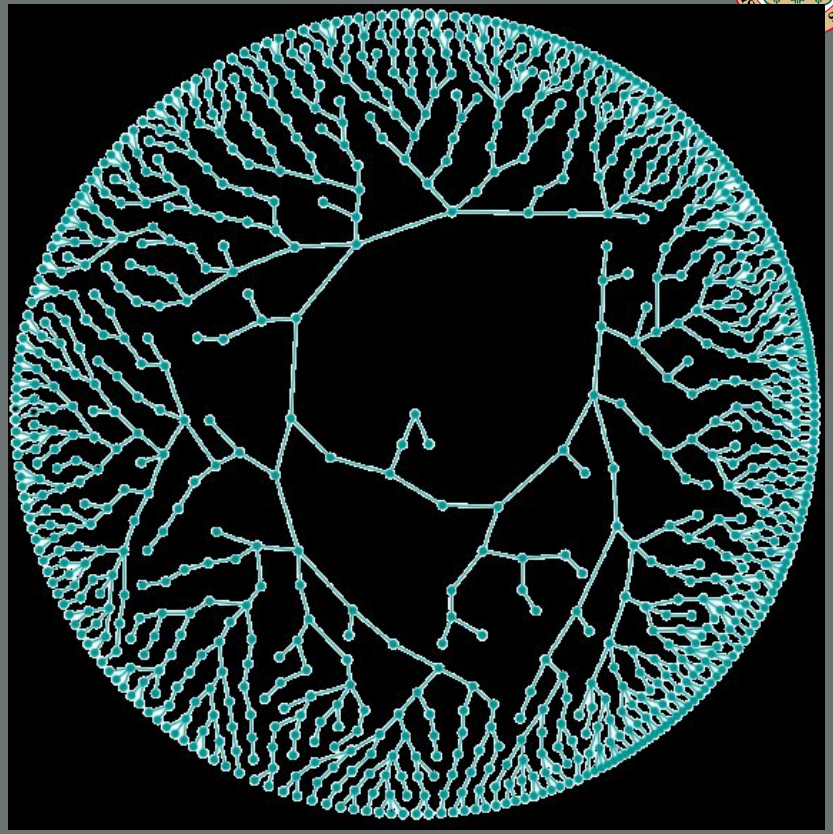
$$W_i = W \times \mathrm{EXP}\{[E_{\mathrm{guess}} - V(\mathbf{R})]\Delta\tau\}$$

Eventually the weights will diverge and be dominated by a few paths

Branching

Markov Monte Carlo Chains

The calculation could be dismantled by large statistical errors due to configurations diffusing into regions that contribute very little to the ground state wave function



COPY a walker N times or KILL it

$$N_i = \mathrm{INT}(|W_i| + \mathrm{RND}[0,1])$$

Skews configurations towards *important* contributions

The “Fermion Sign Problem”

The basic concepts of GFMC

Nucleons are fermions

The wave function must be antisymmetric

Fermionic ground state is an excited state of the bosonic ground state

GFMC will sample the bosonic ground state

Significant cancellation between symmetric and antisymmetric parts

Massive statistical error!

Mitigating the fermion sign problem

A "Constrained-Path" Algorithm

(Zhang, Carlson, Gubernatis 1995)

(Wiringa *et al* 2000)

The constraint

$$\langle \Psi_0(\mathbf{R}) | \Psi_n(\mathbf{R}) \rangle > 0$$

Dismantles variational upper bound

Release the constraint at the end for ~ 20-40 steps

Trade off

Computing Matrix Elements

Using the nearly exact wave function samples

Diagonal

$$\langle \mathcal{O}(\tau) \rangle = \frac{\langle \Psi(\tau) | \mathcal{O} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle} \approx 2 \langle \mathcal{O}(\tau) \rangle_{\text{mixed}} - \langle \mathcal{O} \rangle_{\text{VMC}}$$

Off-diagonal

$$\langle \mathcal{O}(\tau) \rangle \approx \frac{|\Psi^i_{\text{VMC}}|}{|\Psi^f_{\text{VMC}}|} \frac{\langle \Psi^f_{\text{VMC}} | \mathcal{O} | \Psi^i(\tau) \rangle}{\langle \Psi^i_{\text{VMC}} | \Psi^i(\tau) \rangle} + \frac{|\Psi^f_{\text{VMC}}|}{|\Psi^i_{\text{VMC}}|} \frac{\langle \Psi^f(\tau) | \mathcal{O} | \Psi^i_{\text{VMC}} \rangle}{\langle \Psi^f(\tau) | \Psi^f_{\text{VMC}} \rangle} - \langle \mathcal{O} \rangle_{\text{VMC}}$$

Fixed Interior Wave (FIW) Approximation

Normalization

The basics concepts of GFMC

$$\hat{H} - E_{\text{guess}} \longrightarrow E_o = 0$$

Evolving GFMC Scattering States

(Nollett *et al* 2007)

inside outside

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_{12}|<R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R}) + \int_{|\mathbf{r}_>|>R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_> G(\mathbf{R}', \mathbf{R}; \Delta\tau)\Psi_n(\mathbf{R})$$

The contribution of the outside region is mapped to an integral over the interior region by a change of variables

$$\Psi_{n+1}(\mathbf{R}') = \int_{|\mathbf{r}_{12}|<R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} G(\mathbf{R}', \mathbf{R}; \Delta\tau) \times \left[\Psi_n(\mathbf{R}) + \frac{G(\mathbf{R}', \mathbf{R}_>; \Delta\tau)}{G(\mathbf{R}', \mathbf{R}; \Delta\tau)} \left(\frac{r_>}{r}\right)^3 \Psi_n(\mathbf{R}_>)\right]$$

The Change of Variables

Scattering in GFMC

(Nollett *et al* 2

$$d\mathbf{r}_{12} = r_{12}^2 \sin(\theta) dr_{12} d\theta d\phi$$

Need to compute $$\int_{|\mathbf{r}_>|>R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_> G(\mathbf{R}', \mathbf{R}; \Delta\tau) \Psi_n(\mathbf{R})$$

One way to do this ...

$$\mathbf{r}_{12} = \left(\frac{\mathrm{R}_0}{|\mathbf{r}_>|}\right)^2 \mathbf{r}_> \qquad d\mathbf{r}_> = d\mathbf{r}_{12} \left(\frac{|\mathbf{r}_>|}{|\mathbf{r}_{12}|}\right)^3$$

Equivalent to compute $$\int_{|\mathbf{r}_{12}|<R_0} d\mathbf{R}_1 d\mathbf{R}_2 d\mathbf{r}_{12} G(\mathbf{R}', \mathbf{R}_>; \Delta\tau) \left(\frac{|\mathbf{r}_>|}{|\mathbf{r}_{12}|}\right)^3 \Psi_n(\mathbf{R}_>)$$

Enforcing the Boundary Condition

(Nollett *et al* 2007)

Single-Channel (*already done*)

Log-derivative boundary condition + linear extrapolation

$$\Psi_n(\mathbf{R}_>) \approx \left[1 + \zeta_c(\mathbf{R}_> - \mathbf{R}) \cdot \hat{\mathbf{n}}\right] \Psi_n(\mathbf{R})$$