Knowing What We Don't Know: Quantifying Uncertainties in Direct Reaction Theory

Amy Lovell
Michigan State University and
National Superconducting Cyclotron Laboratory

In collaboration with:

Filomena Nunes (MSU/NSCL)

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

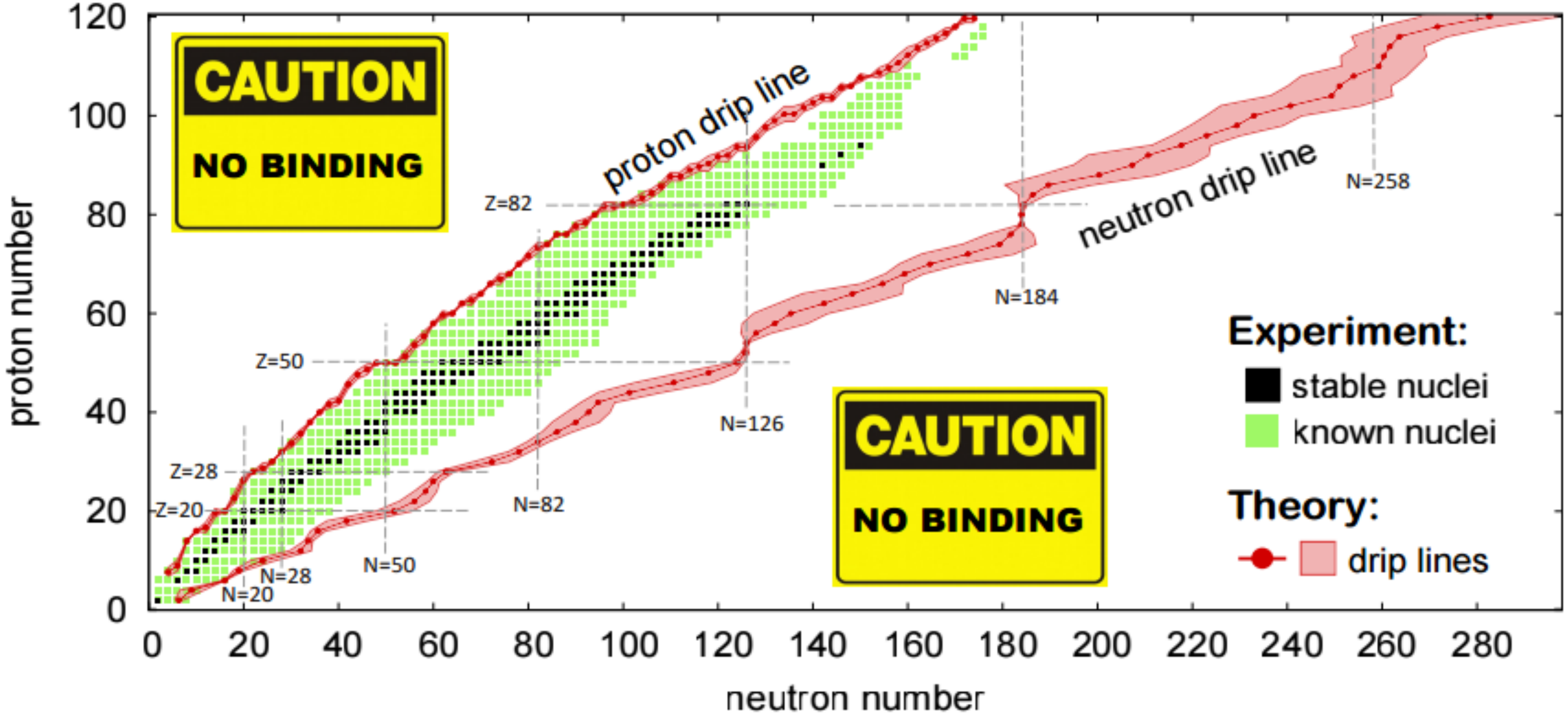
Los Alamos National Laboratory
October 25, 2017

Big Questions in Nuclear Physics

- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technical progress provided by nuclear physics best be used to benefit society?

- Take from *The 2015 Long Range Plan for Nuclear Science*
- *http://science.energy.gov/~/media/np/nsac/pdf/2015LRP/2015_LRPNS_091815.pdf*

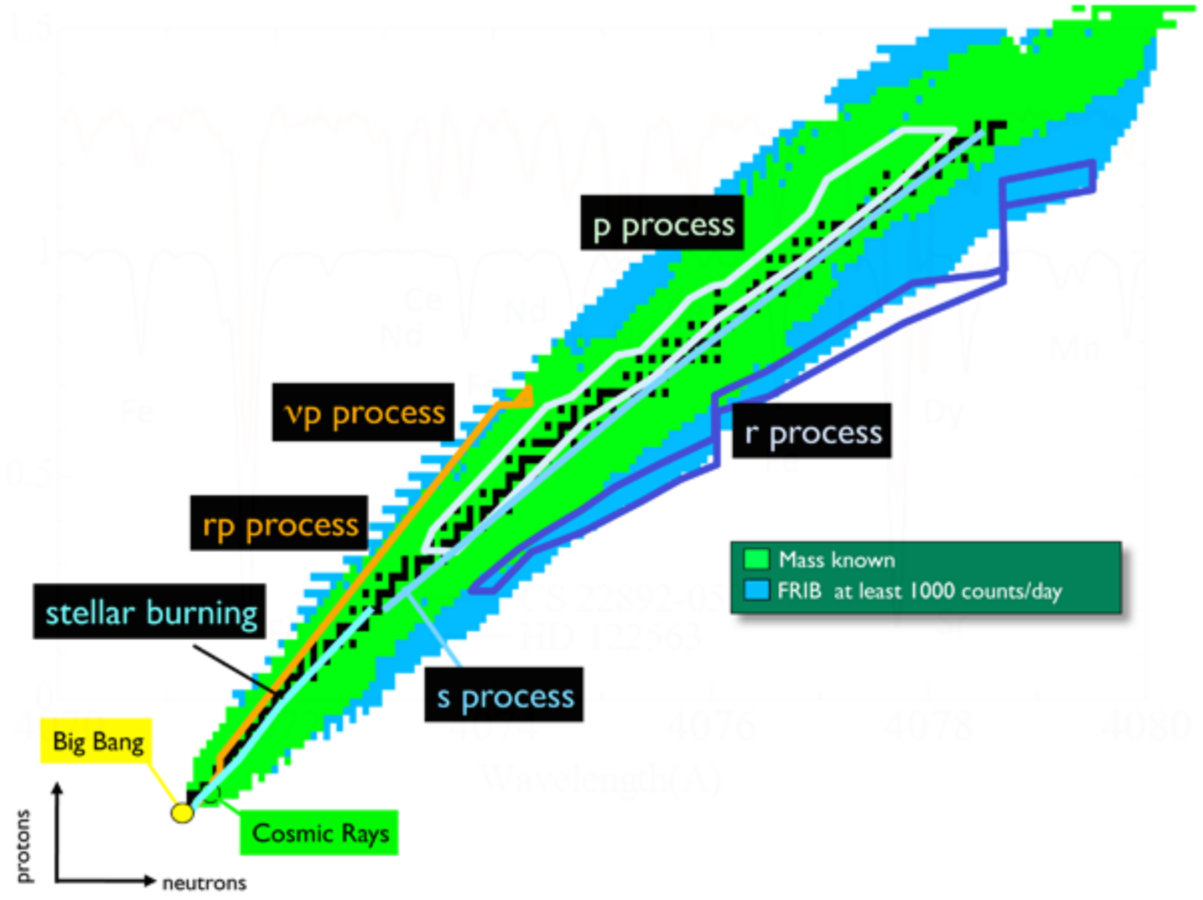
Understanding the Limits of Stability



The 2015 Long Range Plan for Nuclear Science

Understanding the Nuclear Abundances

- Many processes are well known
  - Nuclei involved can be studied directly
- Other nuclei will be only be produced when FRIB comes online (r-process nuclei)
  - These systems are more neutron rich and farther from stability
  - Need indirect measurements to study these systems



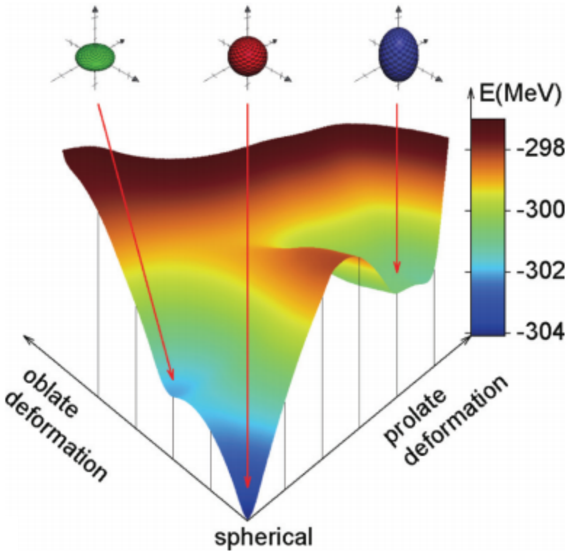
http://www.int.washington.edu/PROGRAMS/14-56w/

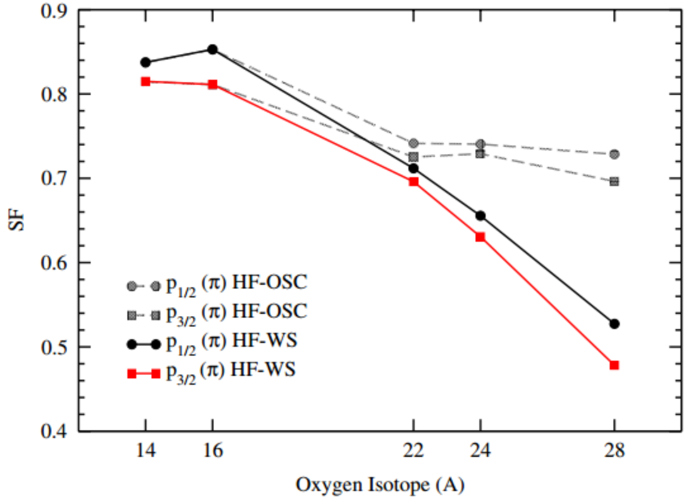
Understanding Properties of Nuclei

How are nuclei shaped?

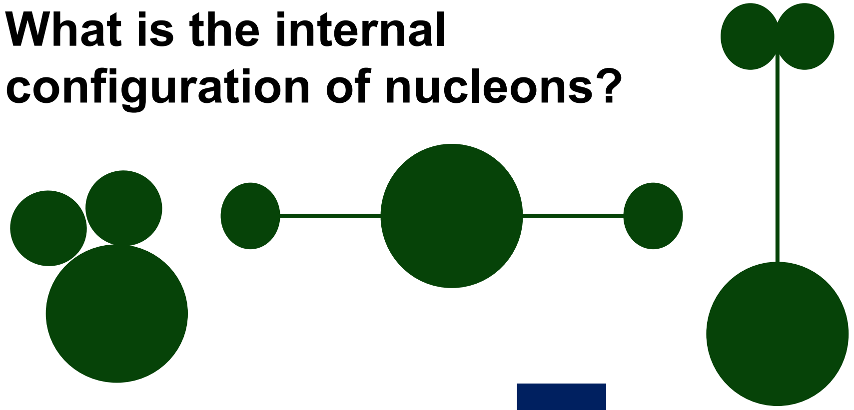
Hartree-Fock calculation for ^{68}Ni

S. Suchyta, et. al., PRC **89** 021301(R) (2014)





What is the internal configuration of nucleons?



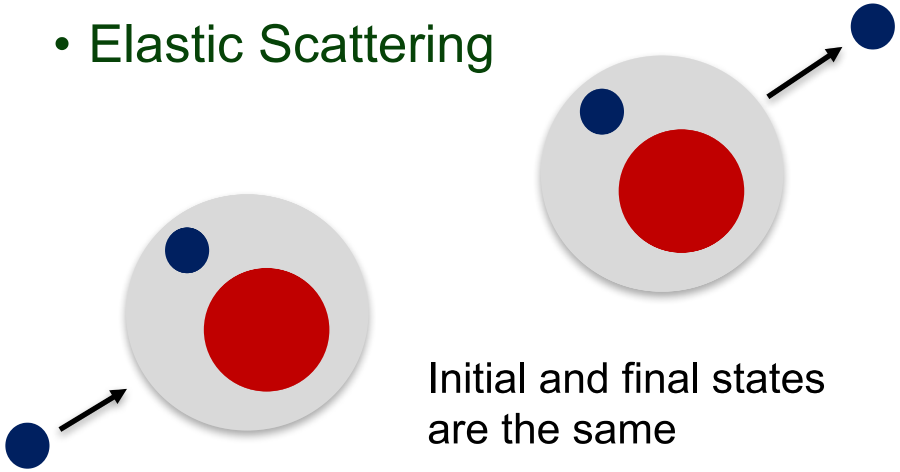
How does the structure of nuclei change away from stability?

O. Jensen, et. al., PRL **107** 032501 (2011)

Can be probed using reactions

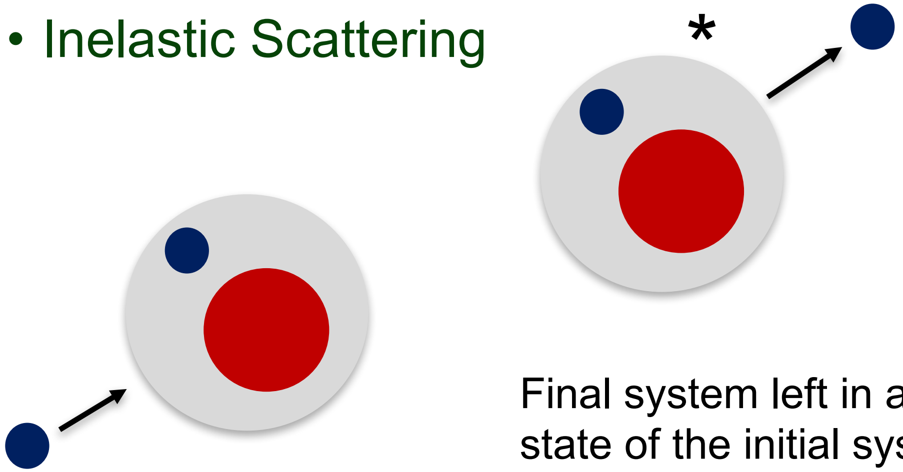
Elastic and Inelastic Scattering

- Elastic Scattering



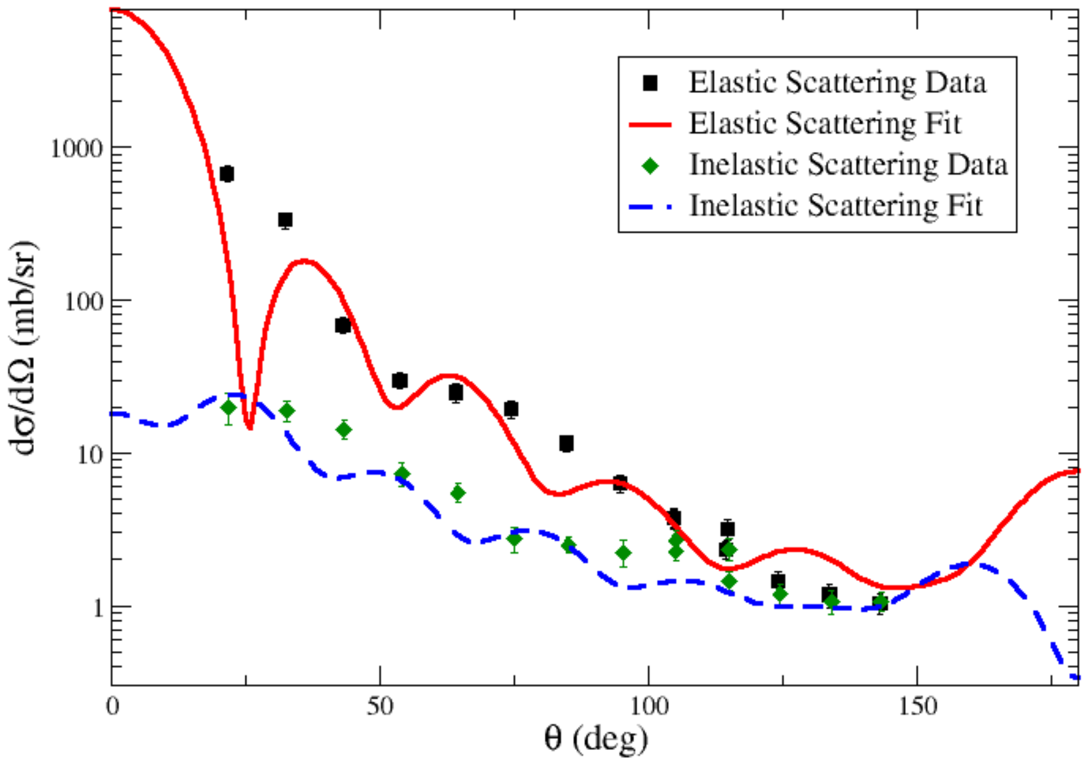
Initial and final states are the same

- Inelastic Scattering



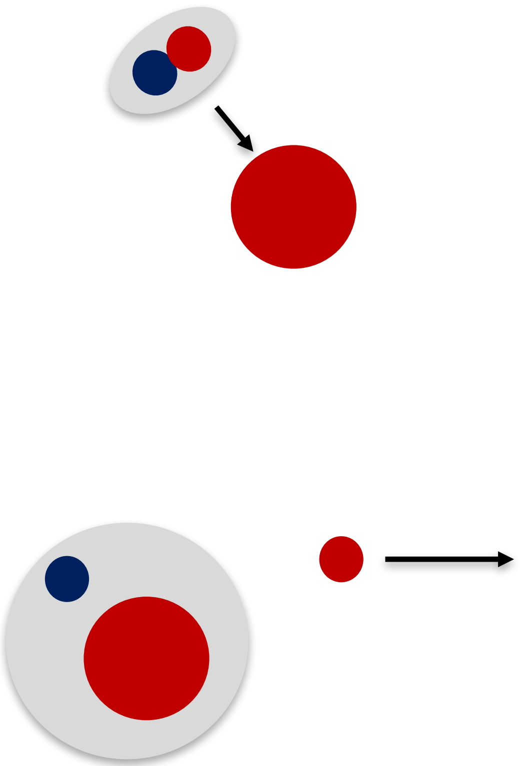
Final system left in an excited state of the initial system

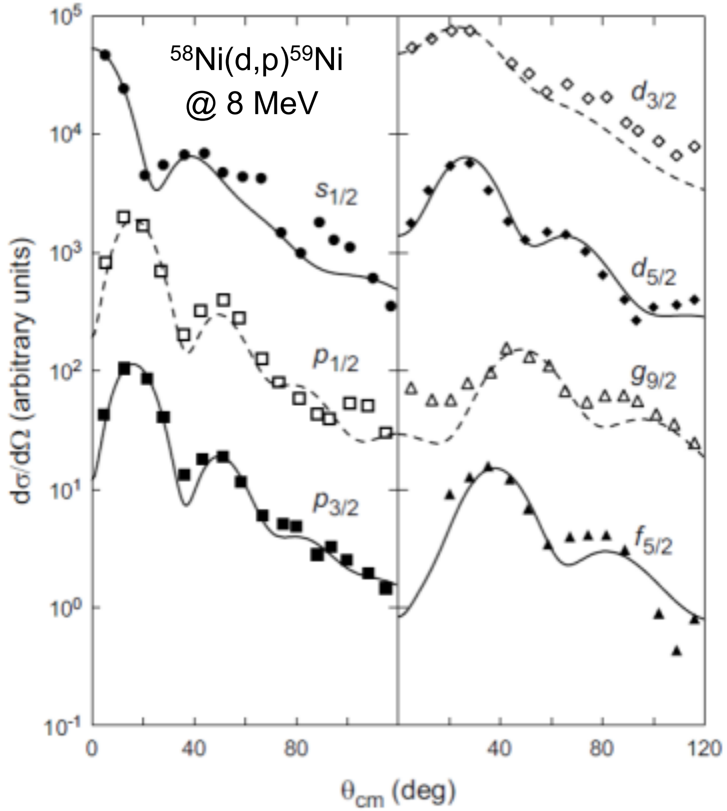
$^{12}C(n,n)^{12}C$ and $^{12}C(n,n^*)^{12}C(2^+_1)$ at 28 MeV



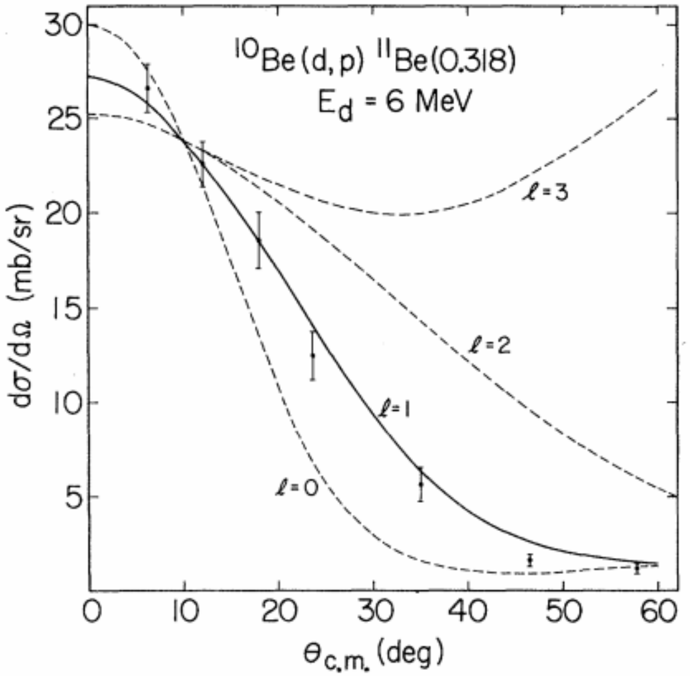
Single Nucleon Transfer Reactions

- Transfer reactions can give information about the states that are being populated





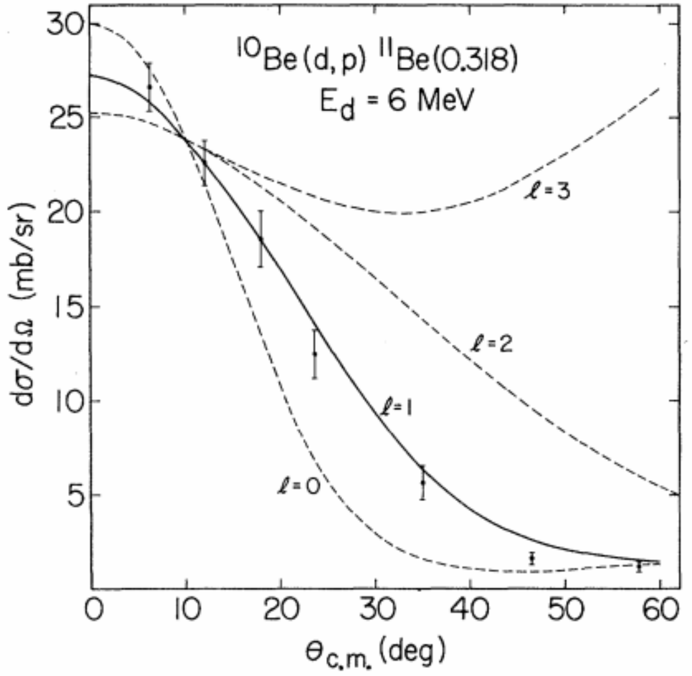
Isotope Science Facility, white paper (2007)



^{10}Be(d,p)^{11}Be @ E_d = 6 MeV

D.R. Goosman and R.W. Kavanagh, PRC 1 1939 (1970)

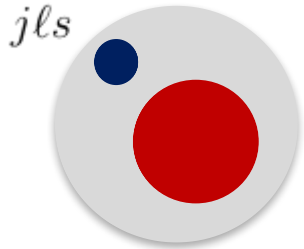
Learning About the Single Particle States in Nuclei

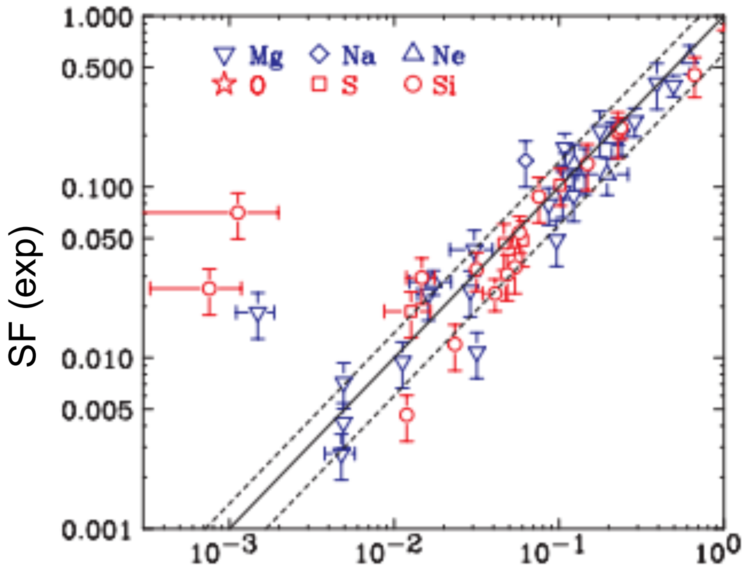


^{10}Be(d,p)^{11}Be @ Ed = 6 MeV

D.R. Goosman and R.W. Kavanagh, PRC 6 1939 (1970)

Calculating spectroscopic factors – probability that a composite nucleus looks like a core plus valence nucleon in a certain configuration



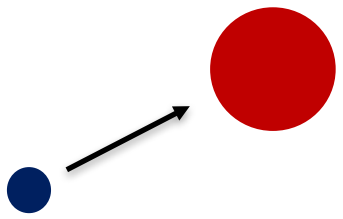


$$\left(\frac{d\sigma}{d\theta}\right)_{\rm exp} = S^{\rm exp}\left(\frac{d\sigma}{d\theta}\right)_{\rm DWBA}$$

$$S^{\rm th} = |\langle\Psi_{A+1}|\Psi_A\rangle|^2$$

M.B. Tsang, et. al., PRL **102** 062501 (2009)

Single Channel Elastic Scattering



Connecting the theory inputs to outputs that can be compared with experiment causes a highly non-linear problem

$$u''_L(R) = \left[\frac{L(L+1)}{R^2} + \frac{2\mu}{\hbar^2}(V(R) - E)\right] u_L(R) \qquad \chi_L(R) = B u_L(R)$$

Connect to the scattering boundary conditions through the R-matrix

$$\chi_L^{ext}(R) = \frac{i}{2}\left[H_L^-(\eta, kR) - \mathbf{S}_L H_L^+(\eta, kR)\right] \qquad \mathbf{R}_L = \frac{1}{a}\frac{\chi_L(a)}{\chi'_L(a)} = \frac{1}{a}\frac{u_L(a)}{u'_L(a)}$$

$$\sigma_L(\eta) = \arg\Gamma(1 + L + i\eta)$$

Theoretical angular distributions can be compared to experiment but connecting back to the potential is not trivial

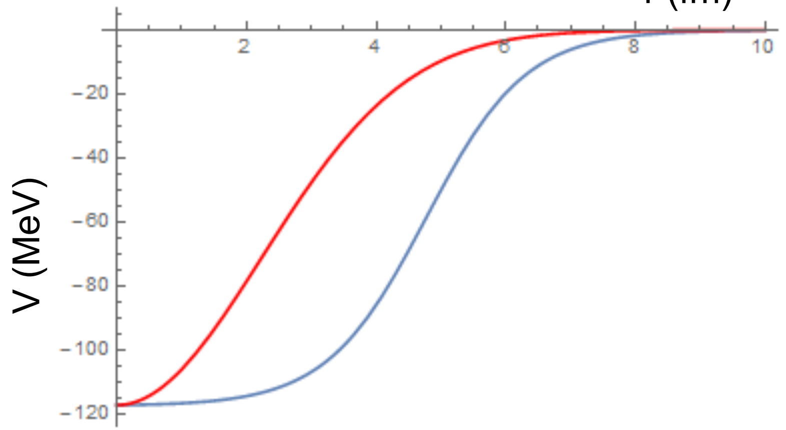
$$\frac{d\sigma}{d\Omega} = \left|\frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)P_L(cos\theta)e^{2i\sigma_L(\eta)}(\mathbf{S}_L - 1)\right|^2 \qquad \eta = \frac{Z_1 Z_2 e^2}{\hbar}\left(\frac{\mu}{2E}\right)^{1/2}$$

I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

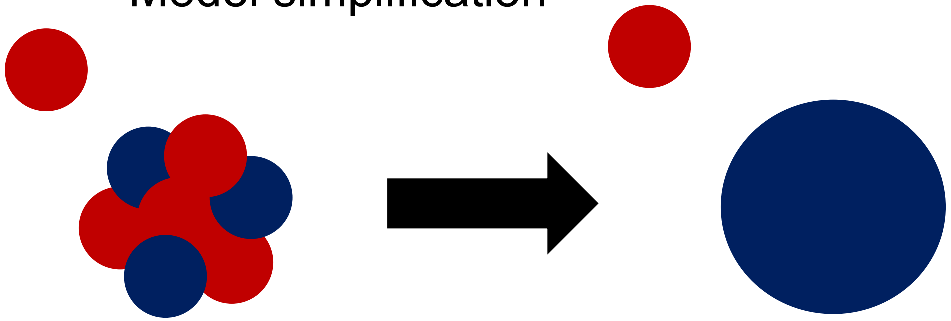
Types of Uncertainties in Reaction Theory

Systematic Uncertainties

Shape of the potential

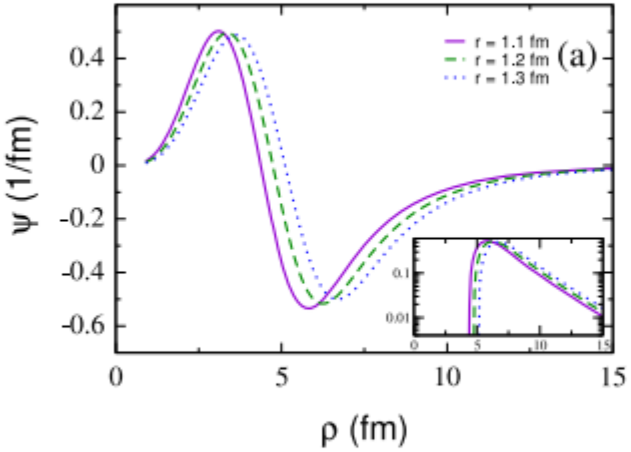


Model simplification



Statistical Uncertainties

Constraints on parameters



Convergence of functions

$$\sum_{k=1}^{k_{max}} f_k(x) \approx \sum_{k=1}^{\infty} f_k(x)$$

A.E. Lovell and F.M. Nunes J. Phys. G **42** 034014 (2015)

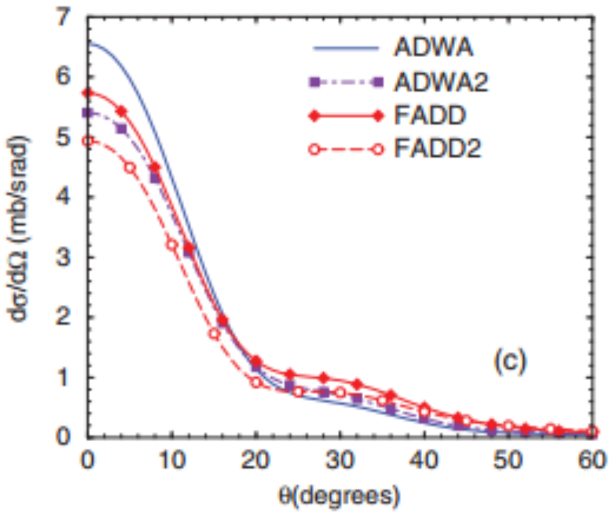
Previously Exploring These Errors

Systematic Uncertainties

Model simplification

$^{12}C(d,p)^{13}C$ at E_d=56 MeV

F.M. Nunes and A. Deltuva, PRC **84** 034607 (2011)



Statistical Uncertainties

Constraints on parameters

Target	E_d (MeV)	θ_{peak}(degrees)	$\frac{d\sigma}{d\Omega}_{peak}^{CH}(\frac{mb}{srad})$	$\frac{d\sigma}{d\Omega}_{peak}^{BG}(\frac{mb}{srad})$	% Error
^{48}Ca	10	14	66.72	61.40	8.30
^{48}Ca	23.2	5	61.25	35.70	55.0
^{132}Sn	9.46	54	7.317	5.931	20.9
^{132}Sn	20	12	24.02	19.31	21.7

$^{48}Ca(d,p)^{49}Ca$ and $^{132}Sn(d,p)^{133}Sn$

A.E. Lovell and F.M. Nunes J. Phys. G **42** 034014 (2015)

Optical Model Parameterizations

- Parameters enter the model in the potential between the nuclei

- Using the Optical Model

$$U(r) = V(r) + iW(r) + (V_{so}(r) + iW_{so}(r))(\mathbf{l}\cdot\mathbf{s}) + V_C(r)$$

Volume Term

$$V(r) = f(r; V_o, R_o, a_o)$$

Surface and Spin-Orbit Terms

$$V(r) = \frac{d}{dr} f(r; V_o, R_o, a_o)$$

$$f(r; V_o, R_o, a_o) = -\frac{V_o}{1 + e^{(r-R_o)/a_o}}$$

$\approx$ 6-12 free parameters

I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

Exploring Bayesian Statistics

$$P(\mathcal{H}|\mathcal{D}) = \frac{P(\mathcal{D}|\mathcal{H})P(\mathcal{H})}{P(\mathcal{D})}$$

H – hypothesis, e.g. model formulation
or choice of free parameters
D – constraining data

$P(\mathcal{H})$ Prior – what is known about the model/parameters before seeing the data

$P(\mathcal{H}|\mathcal{D})$ Posterior – probability that the model/parameters are correct after seeing the data

$P(\mathcal{D})$ Evidence – marginal distribution of the data given the likelihood and the prior

$P(\mathcal{D}|\mathcal{H})$ Likelihood – how well the model/parameters describe the data

S. Andreon and B. Weaver, *Bayesian Methods for the Physical Sciences* (Springer, 2015)

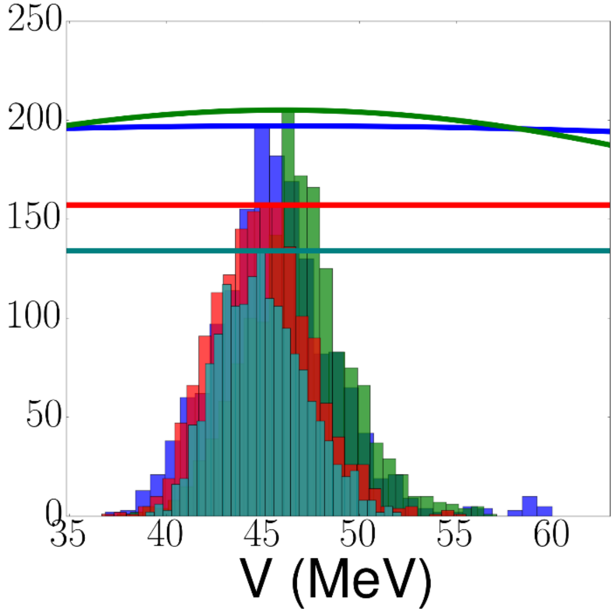
Markov Chain Monte Carlo

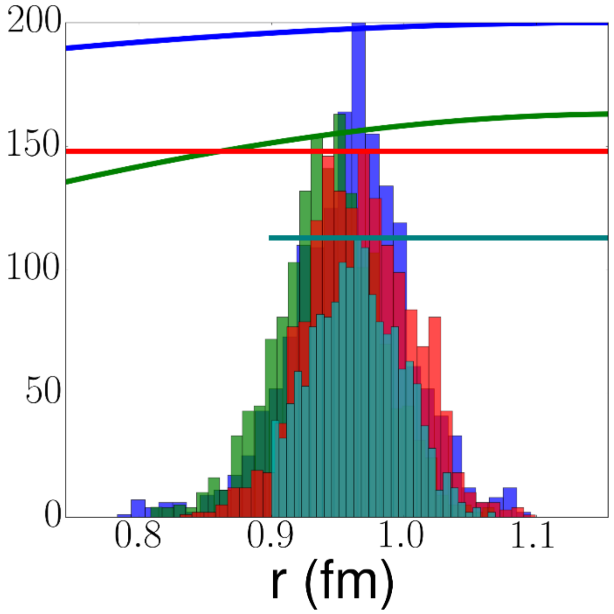
- Using a Metropolis-Hastings Algorithm, where each parameter's step is drawn independently from every other parameter and has a fixed size
- Begin with an initial set of parameters, set the prior, $p(H_i)$, and calculate the likelihood, $p(D|H_i)$
- Randomly choose a new set of parameters, set the prior, $p(H_f)$, and calculate the likelihood, $p(D|H_f)$
- Check the condition: $$\frac{p(H_f)p(D|H_f)}{p(H_i)p(D|H_i)} > R$$
- If the condition is fulfilled, accept the new set of parameters and use these as the initial parameter set
- Otherwise, discard the new parameter set and randomly choose another new set of parameters

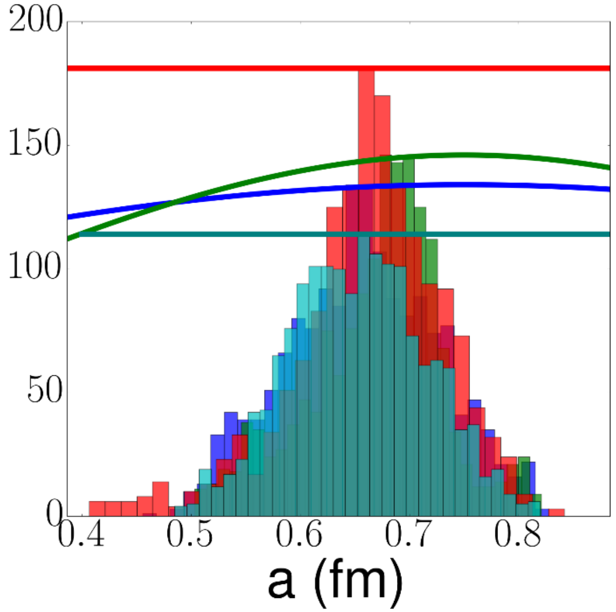
- Dependence on the burn-in length, step size in parameter space, and prior choice

Verifying the Prior Shape
Real Volume Parameters

$^{90}Zr(n,n)^{90}Zr$ at 24.0 MeV



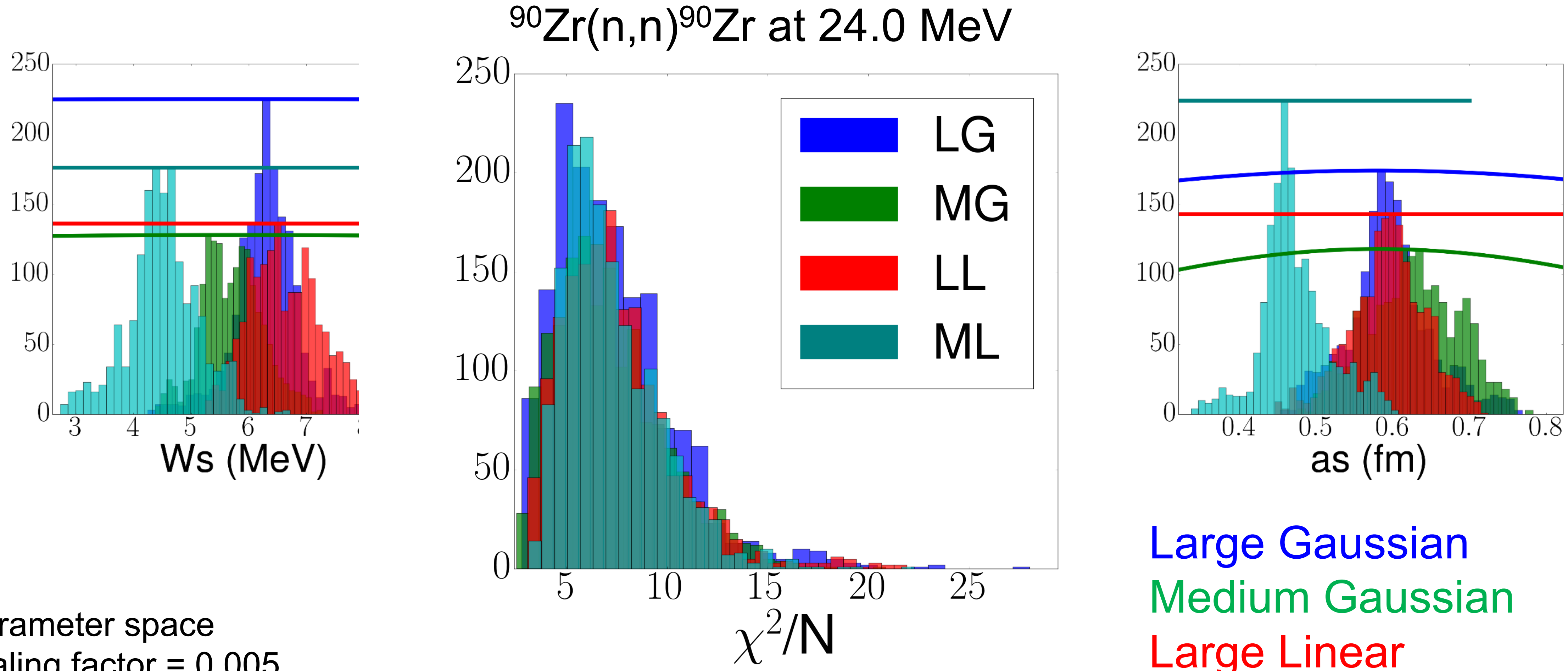




Large Gaussian
Medium Gaussian
Large Linear
Medium Linear

Parameter space
scaling factor = 0.005

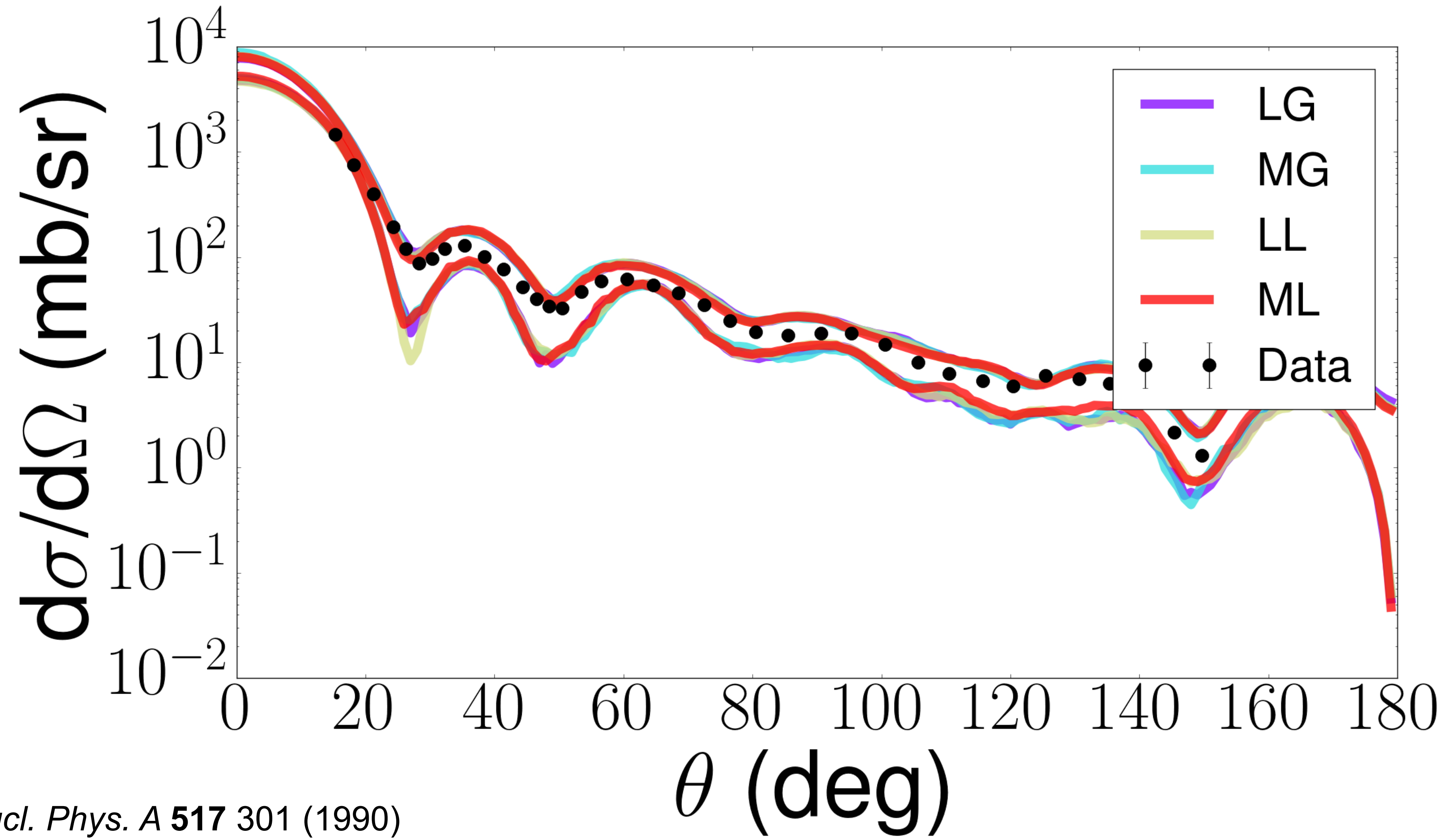
Verifying the Prior Shape
Imaginary Surface Parameters



Parameter space
scaling factor = 0.005

Large Gaussian
Medium Gaussian
Large Linear
Medium Linear

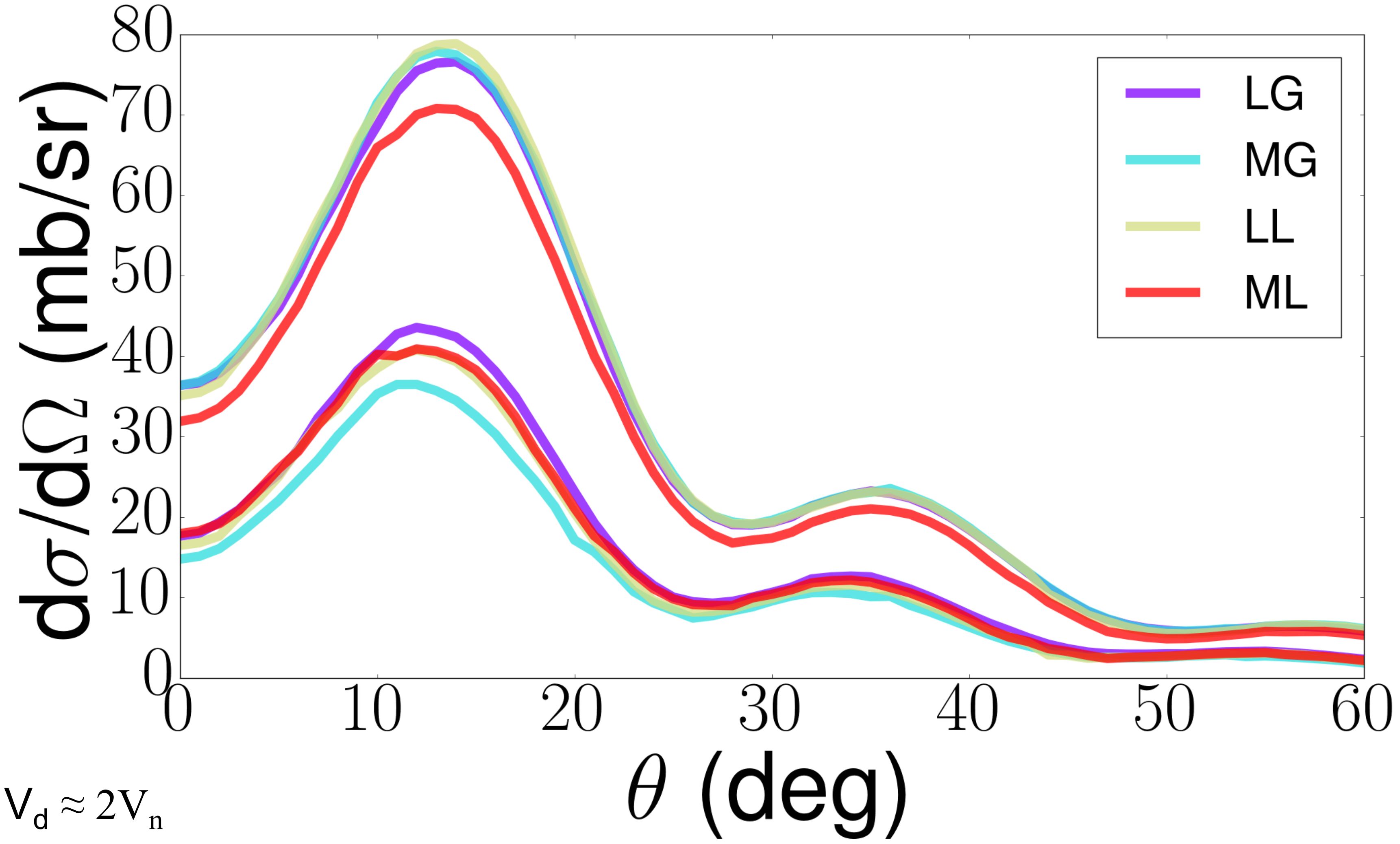
Comparing Elastic Scattering
$^{90}Zr(n,n)^{90}Zr$ at 24.0 MeV



95% confidence intervals

Data from: *Nucl. Phys. A* **517** 301 (1990)

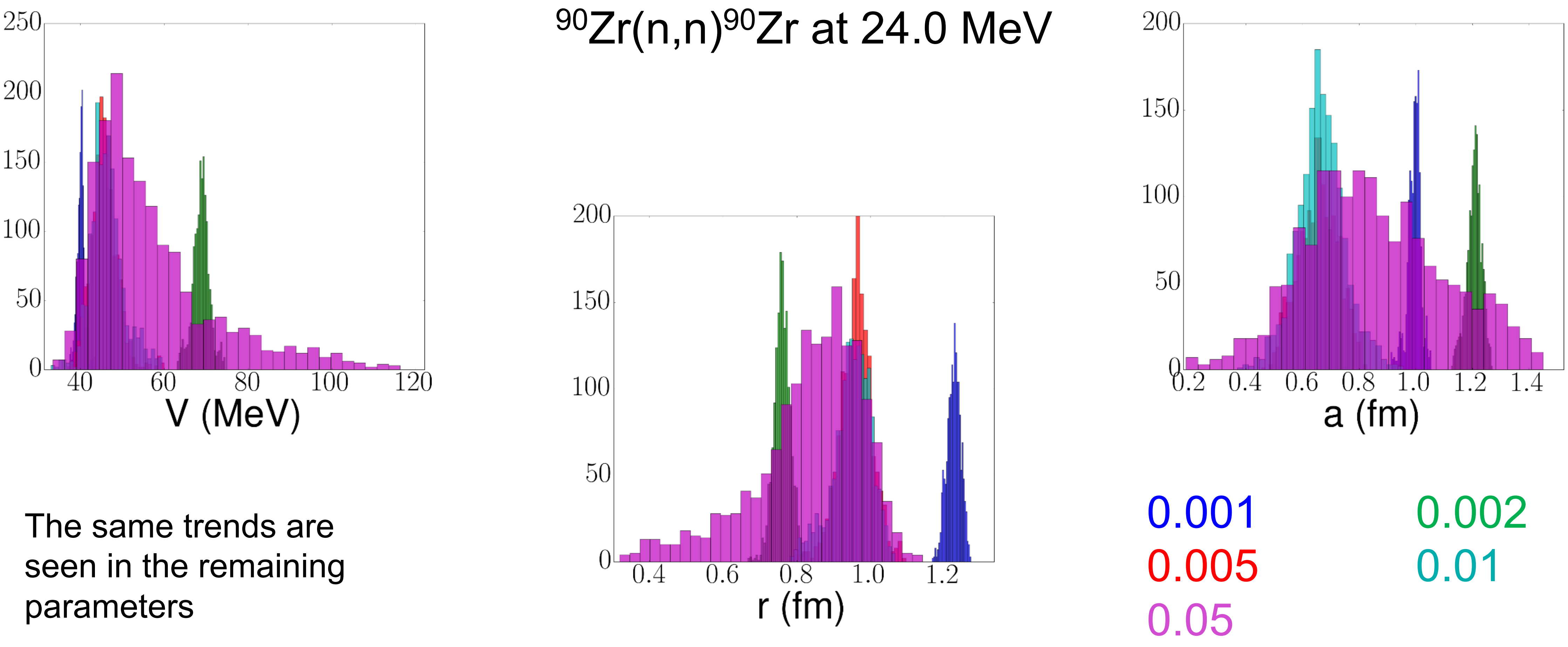
Comparing Transfer Cross Sections
$^{90}Zr(d,p)^{91}Zr$ at 24.0 MeV



95% confidence intervals

DWBA where $V_d \approx 2V_n$

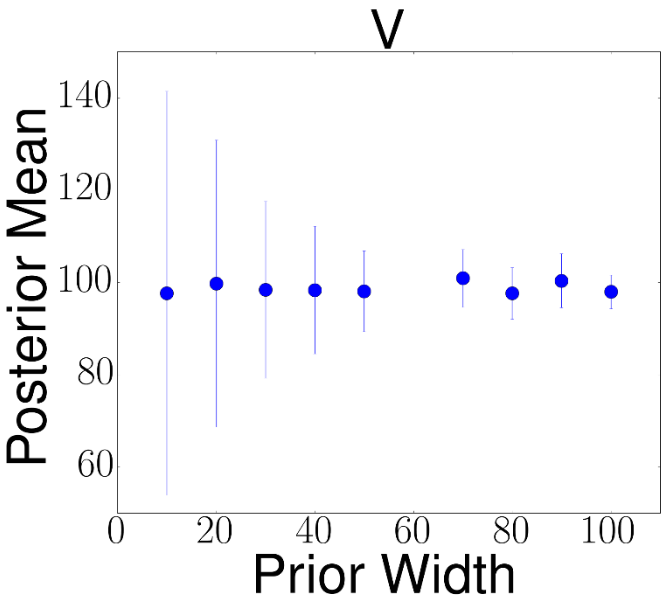
Verifying the Scaling Factor Using the Large Gaussian Prior

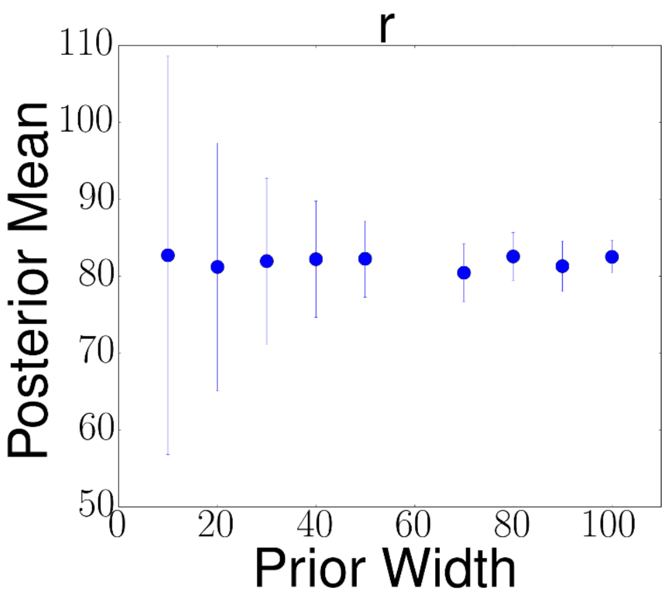


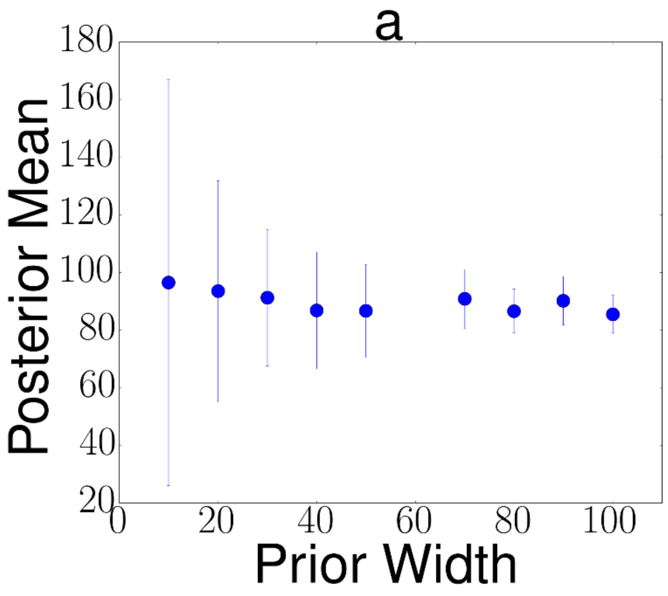
The same trends are seen in the remaining parameters

Systematically Studying Prior Widths with Gaussian Priors

$^{90}Zr(n,n)^{90}Zr$ at 24.0 MeV

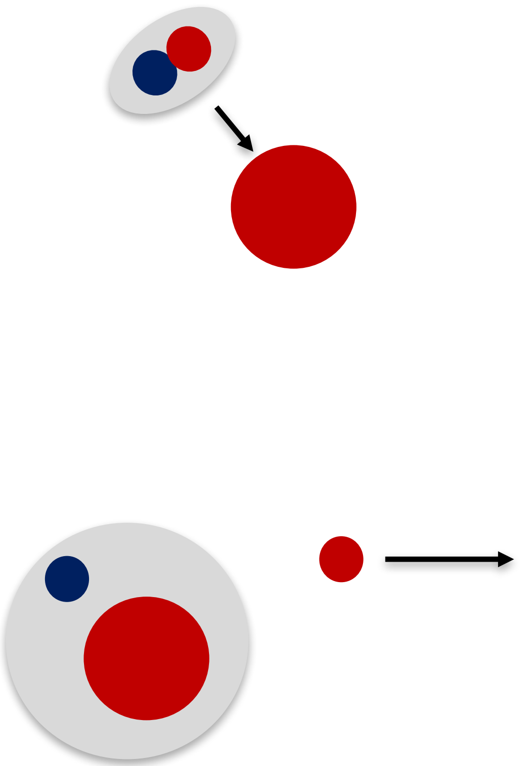


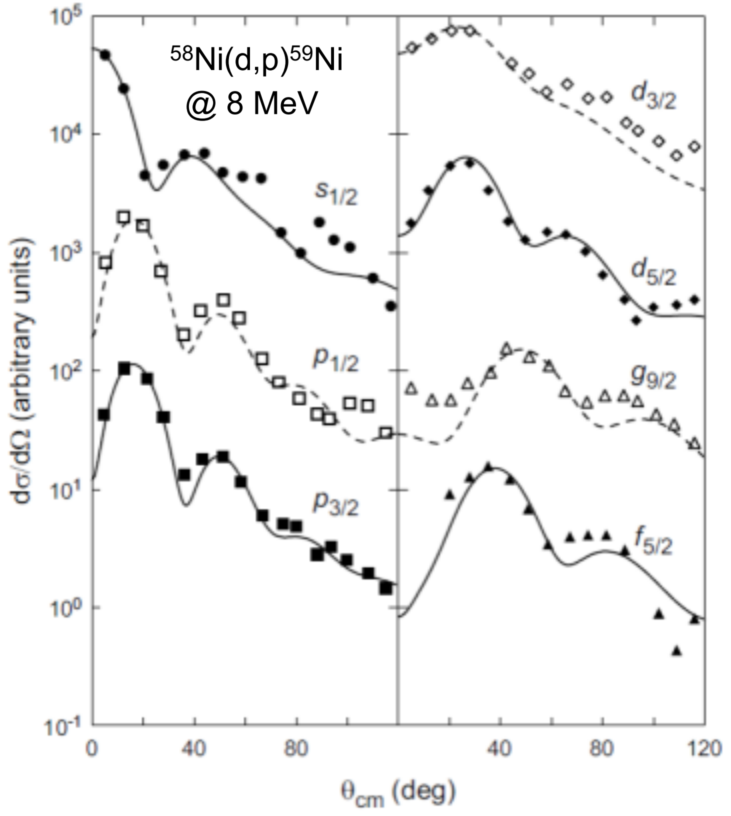




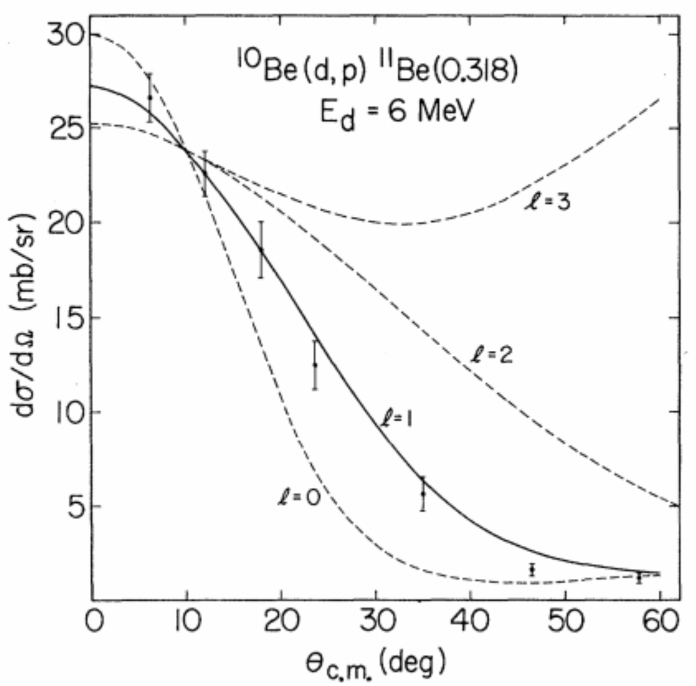
Ultimately Interested in Single Nucleon Transfer Reactions

- Transfer reactions can give information about the states that are being populated





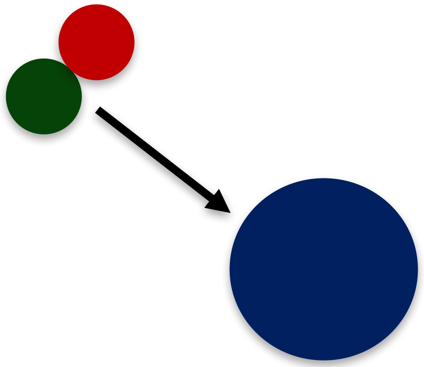
Isotope Science Facility, white paper (2007)



$^{10}Be(d,p)^{11}Be$ @ E_d = 6 MeV

D.R. Goosman and R.W. Kavanagh, PRC 1 1939 (1970)

Reactions Using the Adiabatic Wave Approximation (ADWA)



$$[T_R + \epsilon_0 + V_{bA} + VvA - E]\, \Psi^{\mathrm{ad}}(\vec{r}, \vec{R}) = 0$$

$$\Psi^{\mathrm{ad}}(\vec{r}, \vec{R}) = \phi_0(\vec{r})\chi_0^{\mathrm{ad}}(\vec{R}) + \sum_{i>0} \phi_i(\vec{r})\chi_i^{\mathrm{ad}}(\vec{R})$$

Elastic scattering

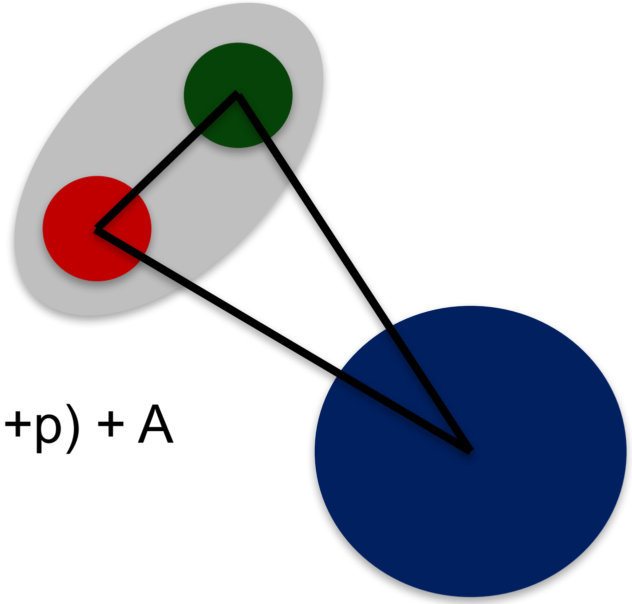
Breakup components

Explicitly takes into account the breakup of the deuteron – through nucleon-target potentials

I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

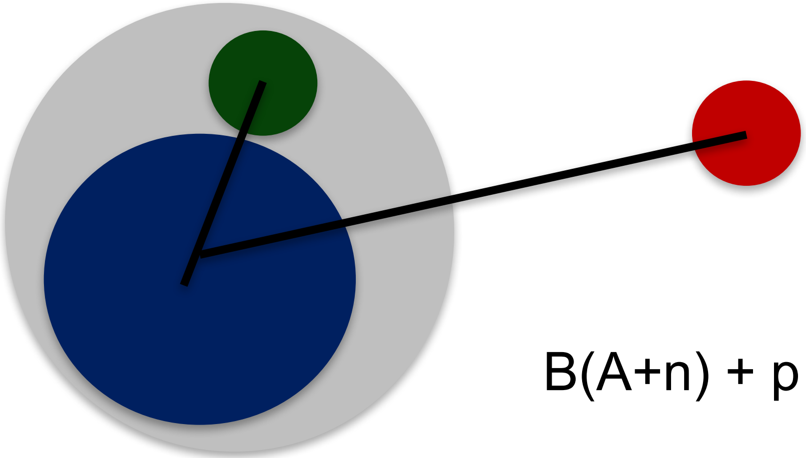
Constraining Nucleon Potentials A(d,p)B

Incoming channel



d(n+p) + A

Outgoing channel

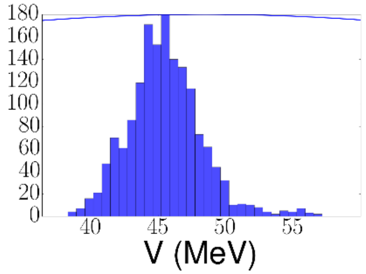


B(A+n) + p

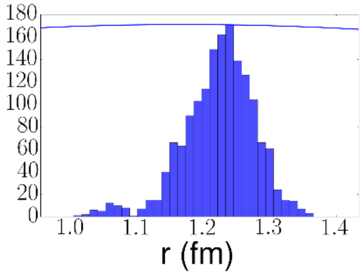
$$T^{(d,p)} = \langle \phi_{An} \chi_p | V_{np} | \phi_d \chi_d^{ad} \rangle$$

^{48}Ca(n,n) at 12.0 MeV
Posterior Distributions

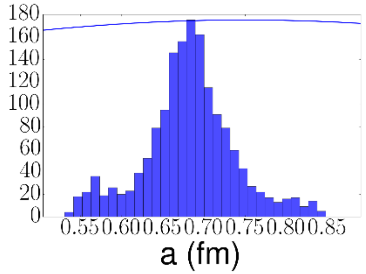
Real Volume



μ=45.51
σ=2.74

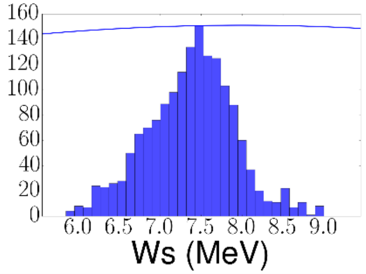


1.22
0.05

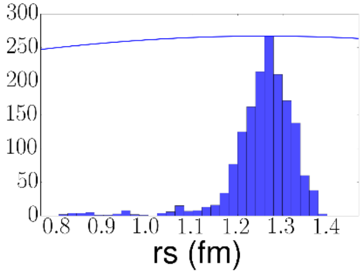


0.68
0.06

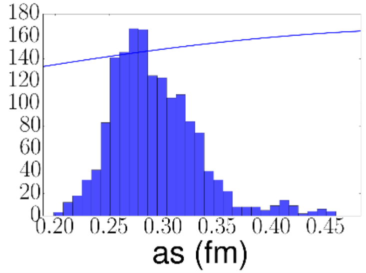
Imaginary Surface



7.38
0.54

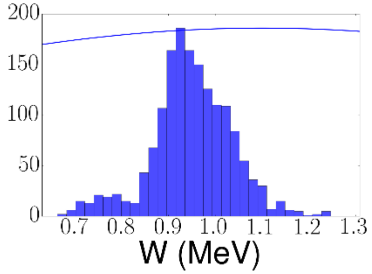


1.25
0.08

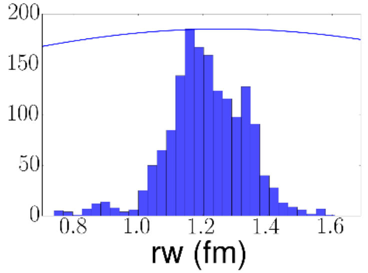


0.29
0.04

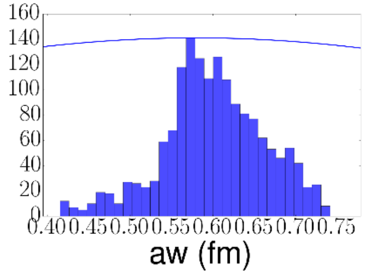
Imaginary Volume



0.95
0.09

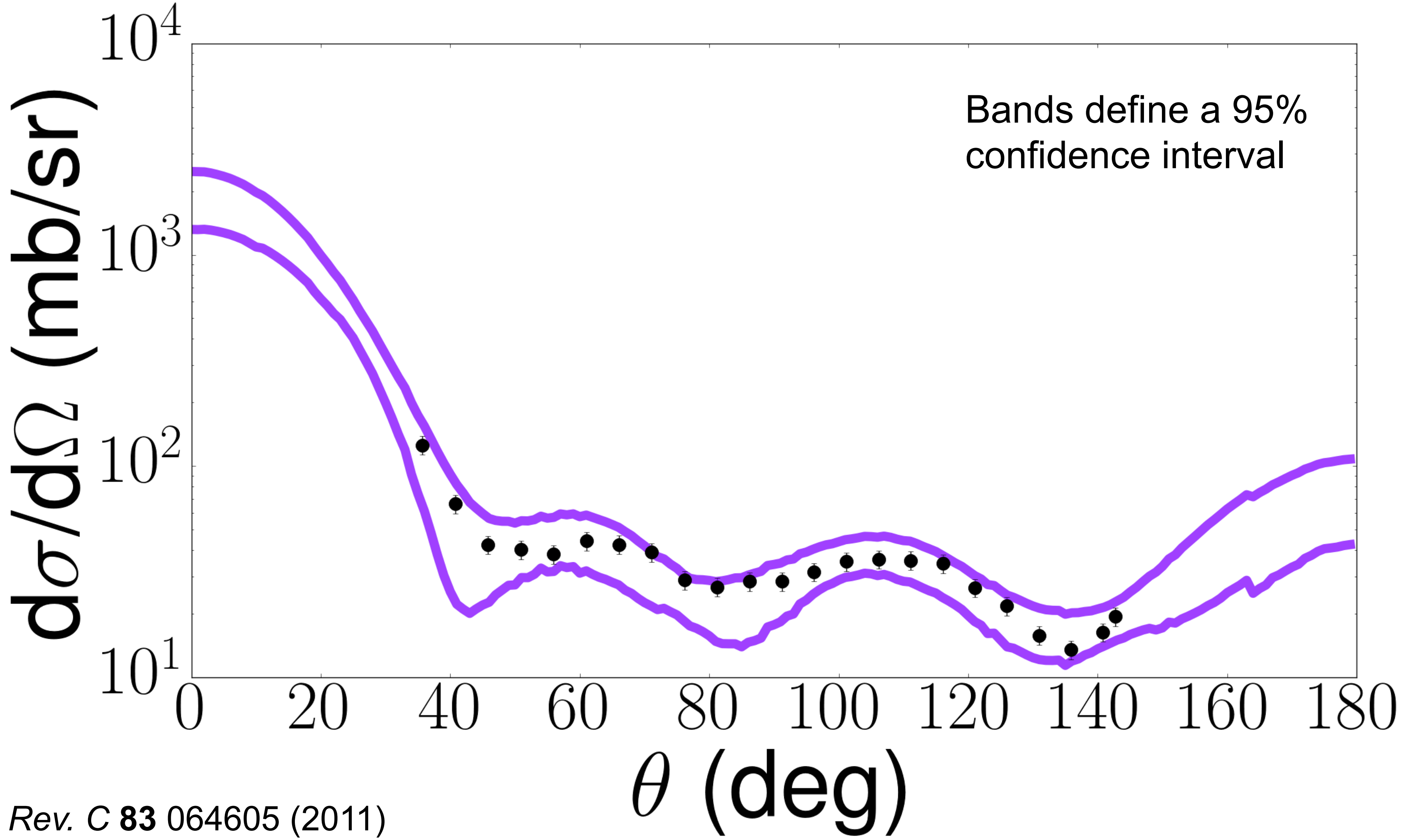


1.21
0.12



0.60
0.06

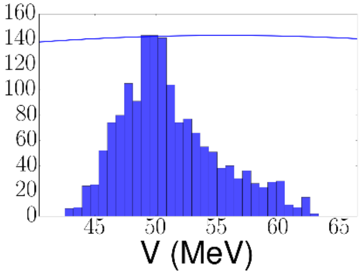
$^{48}Ca(n,n)$ at 12.0 MeV Angular Distribution



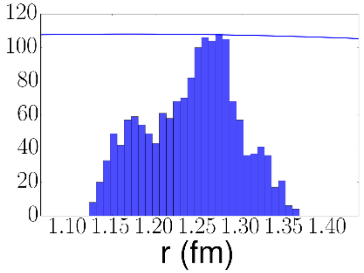
Data from: *Phys. Rev. C* **83** 064605 (2011)

^{48}Ca(p,p) at 14.08 MeV
Posterior Distributions

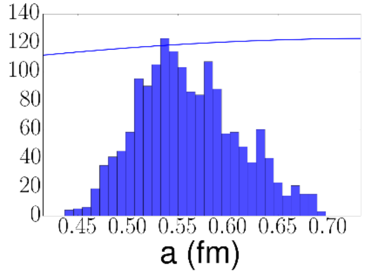
Real Volume



μ=51.15
σ=4.04

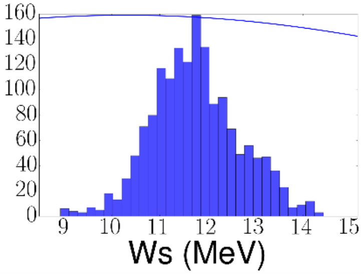


1.24
0.05

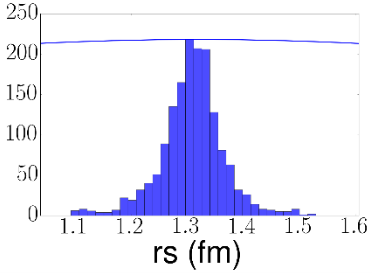


0.56
0.05

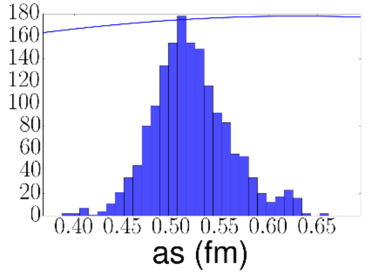
Imaginary Surface



11.75
0.92

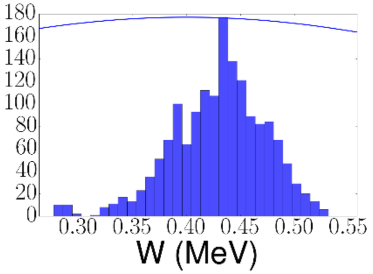


1.31
0.06

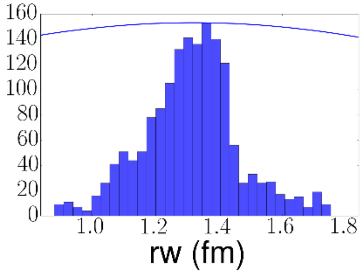


0.52
0.04

Imaginary Volume



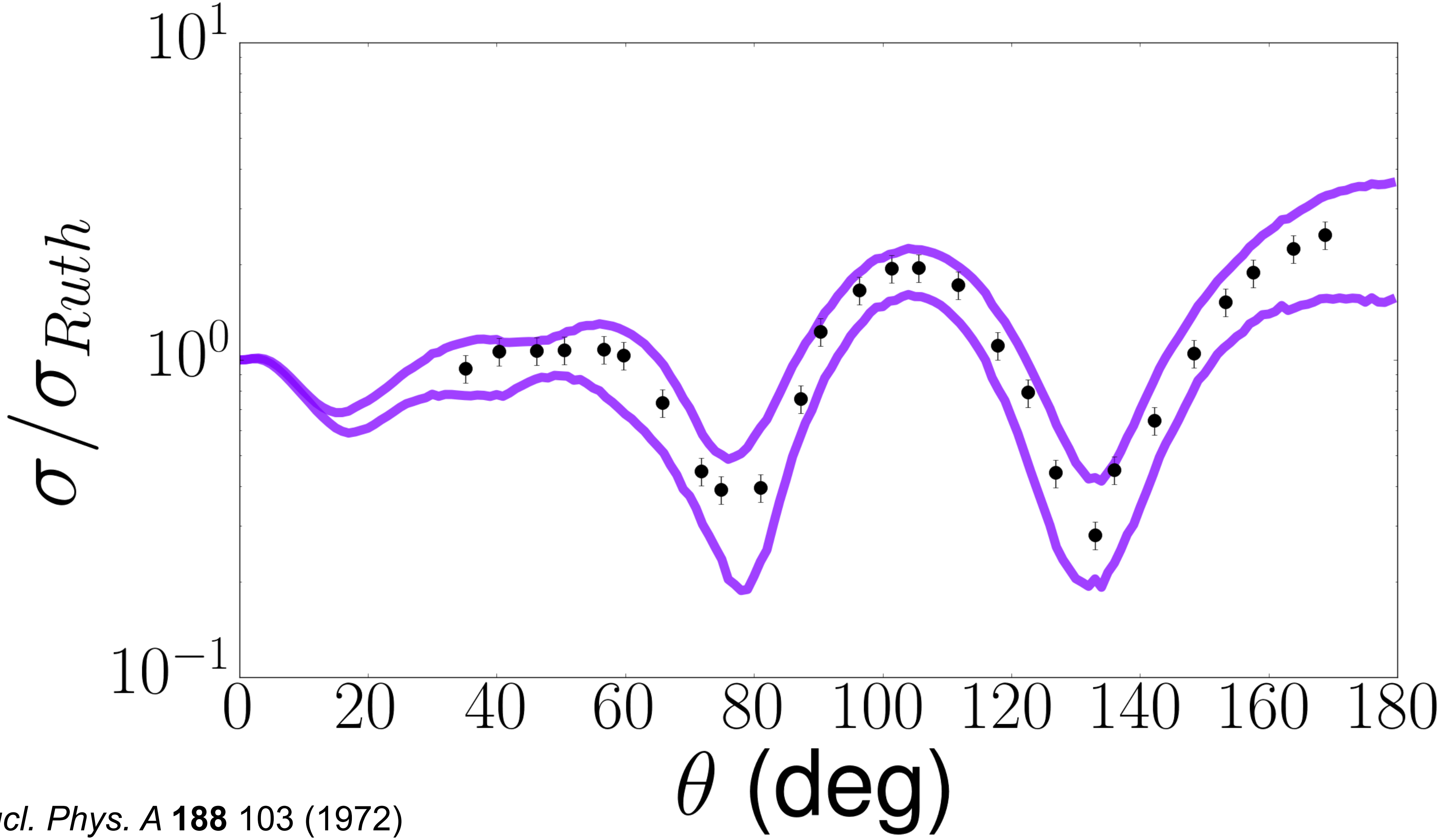
0.43
0.04



1.31
0.15

aw

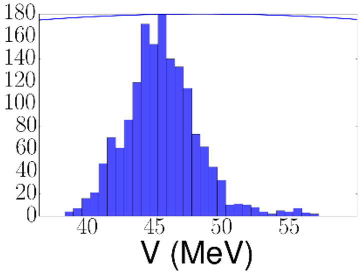
$^{48}Ca(p,p)$ at 14.08 MeV Angular Distribution



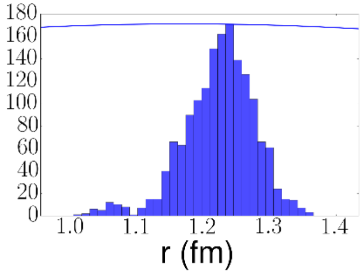
Data from: *Nucl. Phys. A* **188** 103 (1972)

^{48}Ca(p,p) at 25.0 MeV
Posterior Distributions

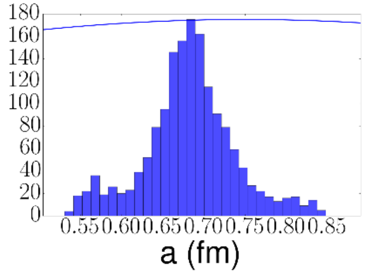
Real Volume



μ=53.49
σ=4.19

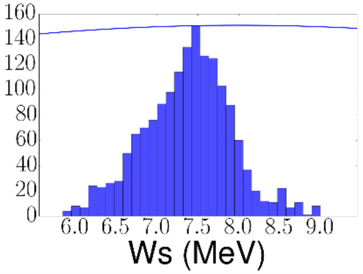


1.14
0.05

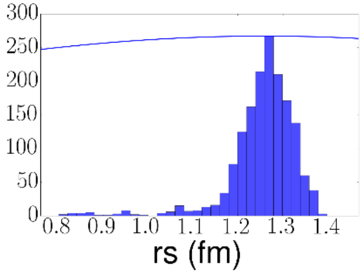


0.73
0.06

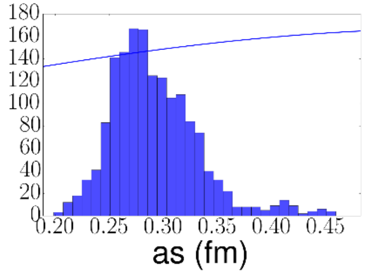
Imaginary Surface



6.82
0.55

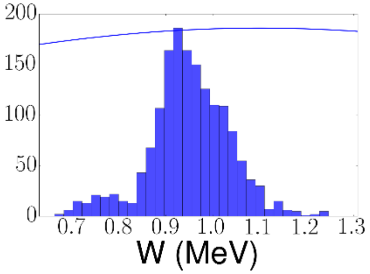


1.33
0.07

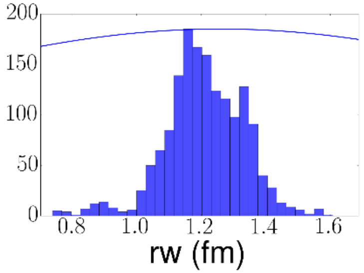


0.59
0.05

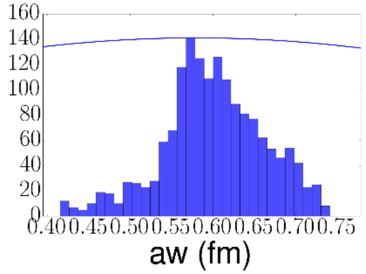
Imaginary Volume



2.25
0.33

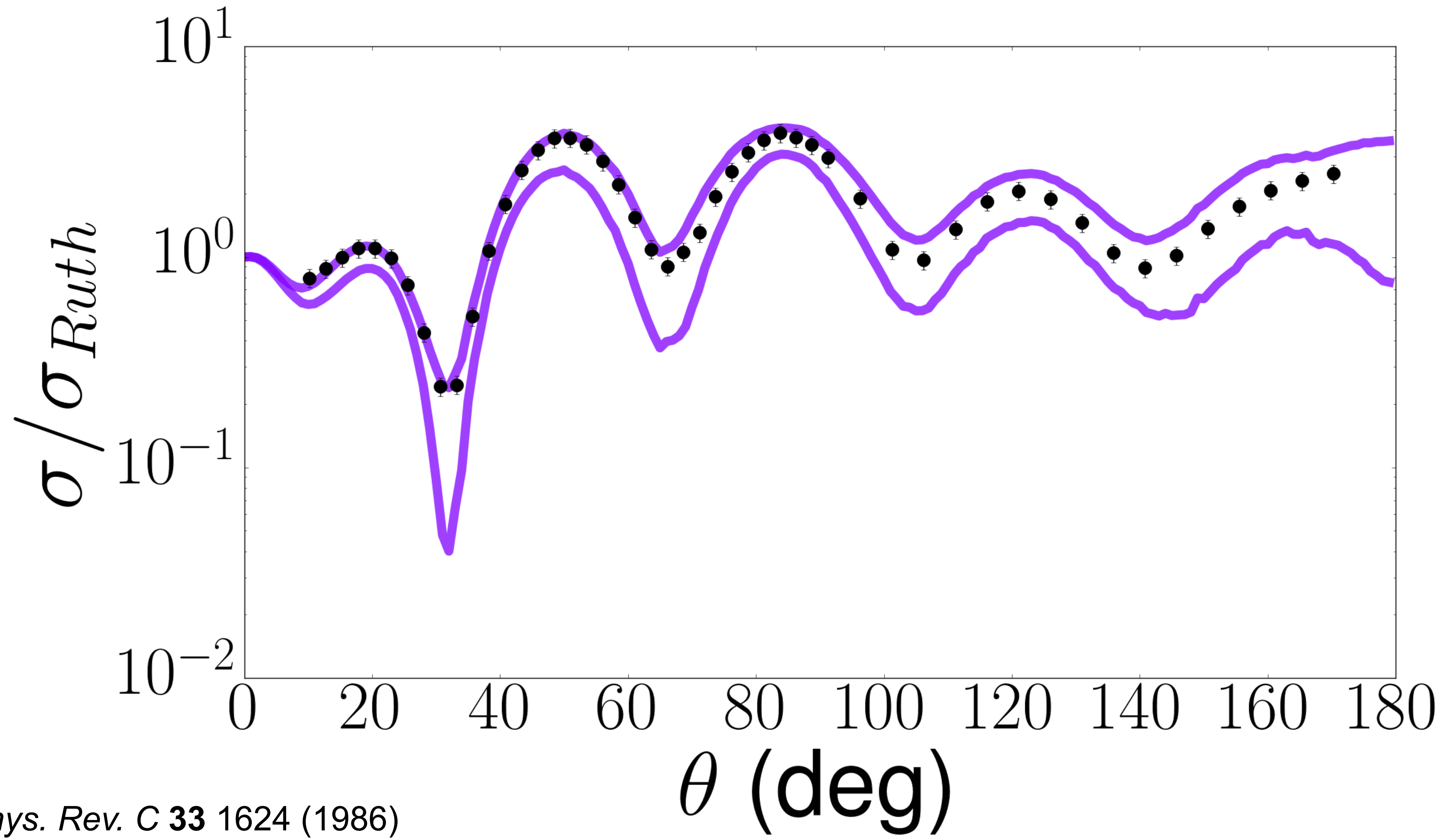


1.28
0.13



0.61
0.07

^{48}Ca(p,p) at 25.0 MeV Angular Distribution



Data from: *Phys. Rev. C* **33** 1624 (1986)

Constructing Transfer Cross Sections

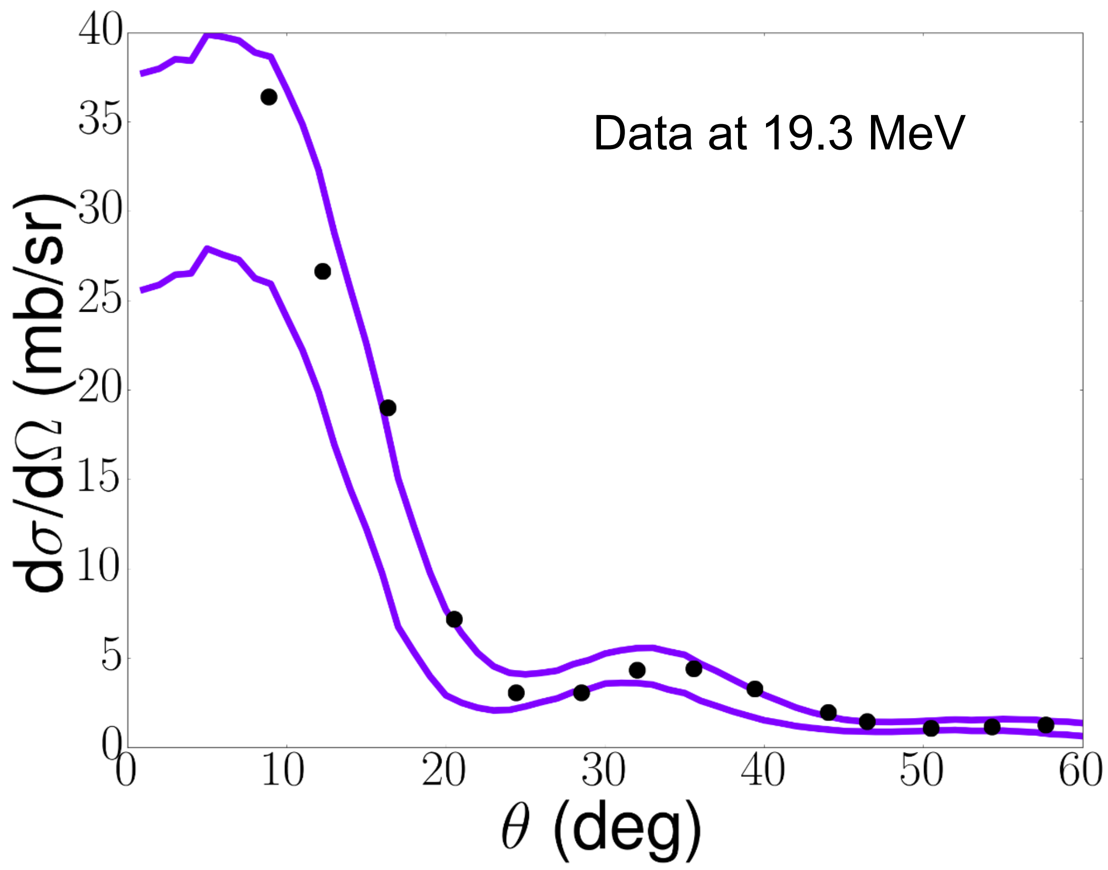
$$T^{(d,p)} = \langle \phi_{An} \chi_p | V_{np} | \phi_d \chi_d^{ad} \rangle$$

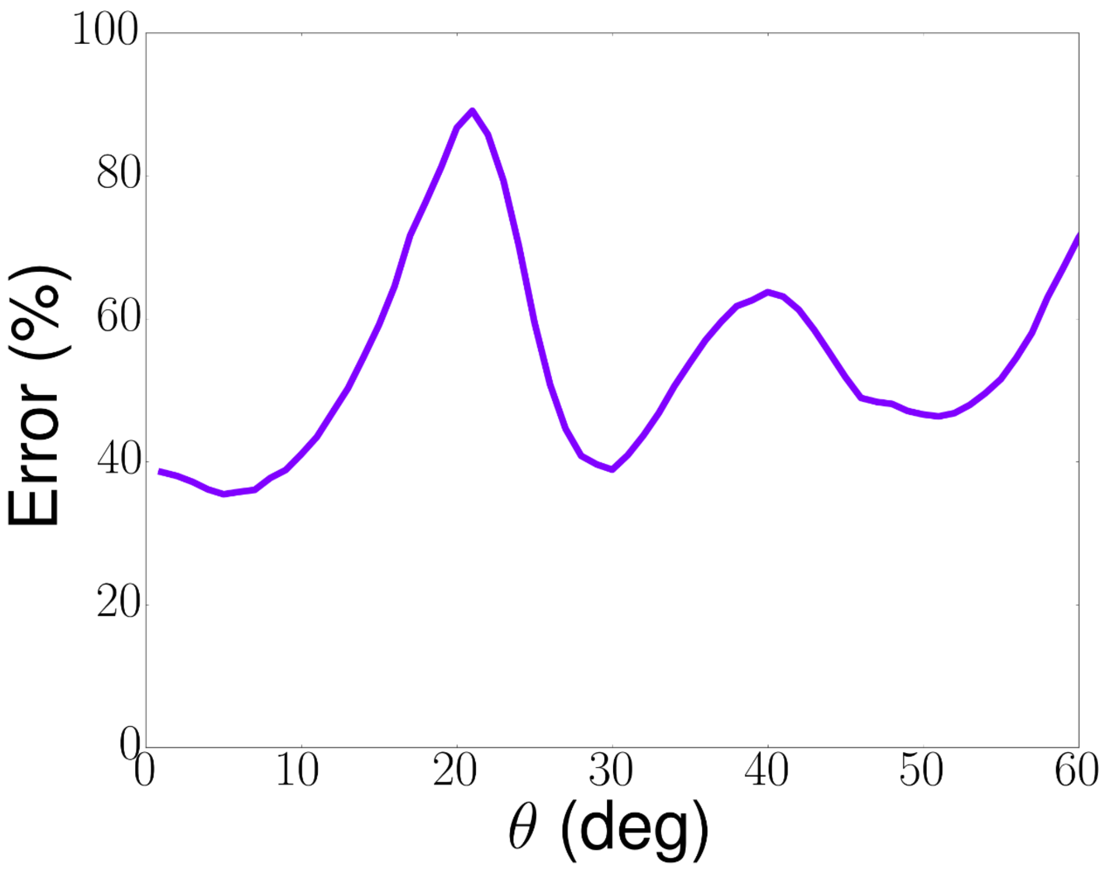
Constrained from ^{48}Ca(p,p) @ 25.0 MeV data

Constrained from ^{48}Ca(p,p) @ 14.03 MeV and ^{48}Ca(n,n) @ 12 MeV data

Posterior distributions are then used to construct PREDICTED distributions for the transfer reaction

^{48}Ca(d,p)^{49}Ca(g.s.) at 24.0 MeV in ADWA

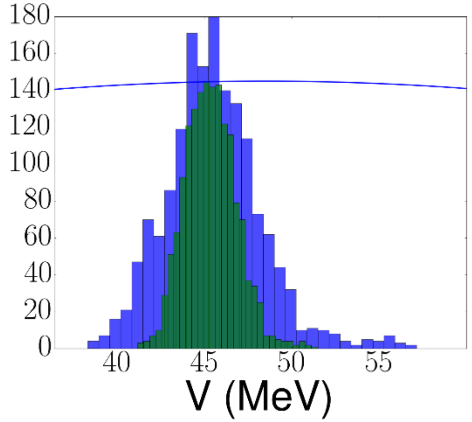


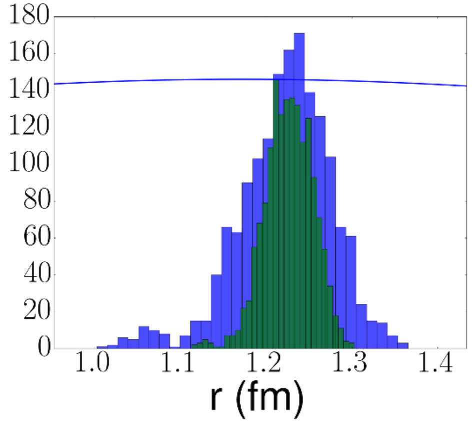


Data extracted from: A.M. Mukhamedzhanov,
F.M. Nunes, and P. Mohr, PRC **77** 051601 (2008)

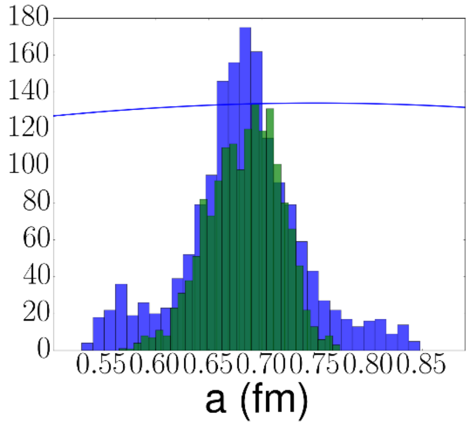
Studying Experimental Error Reduction

$^{48}Ca(n,n)$ at 12.0 MeV





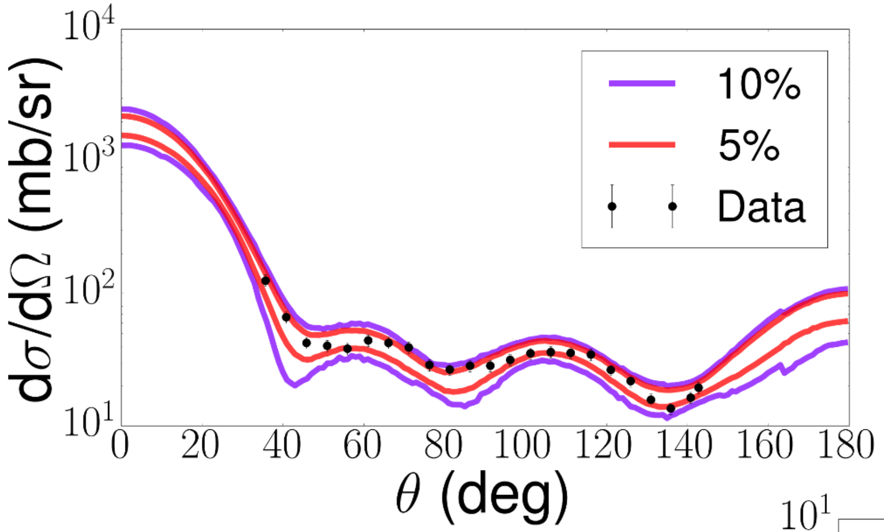
Real Volume



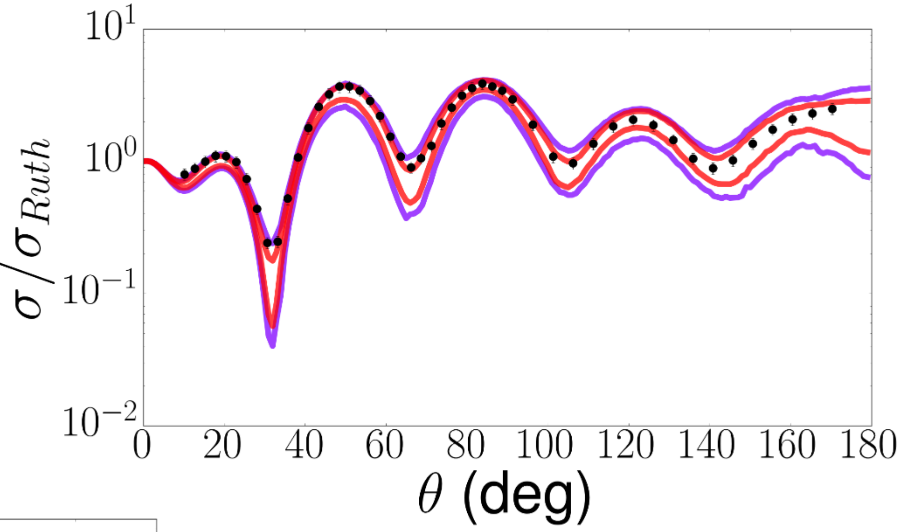
	10% Mean	10% Width	5% Mean	5% Width
V	45.51	2.74	45.35	1.47
r	1.22	0.05	1.23	0.03
a	0.68	0.06	0.68	0.03
Ws	7.38	0.54	6.80	0.59
rs	1.25	0.08	1.26	0.04
as	0.29	0.04	0.31	0.03
W	0.95	0.09	1.01	0.11
r	1.21	0.12	1.13	0.15
a	0.60	0.06	0.62	0.05

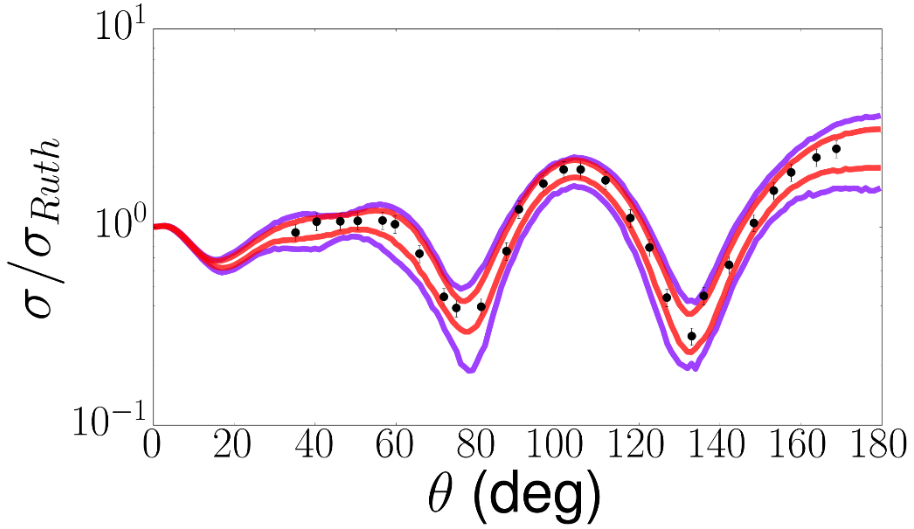
Error Reduction in the Elastic Cross Sections

^{48}Ca(n,n) at 12.0 MeV



^{48}Ca(p,p) at 14.03 MeV

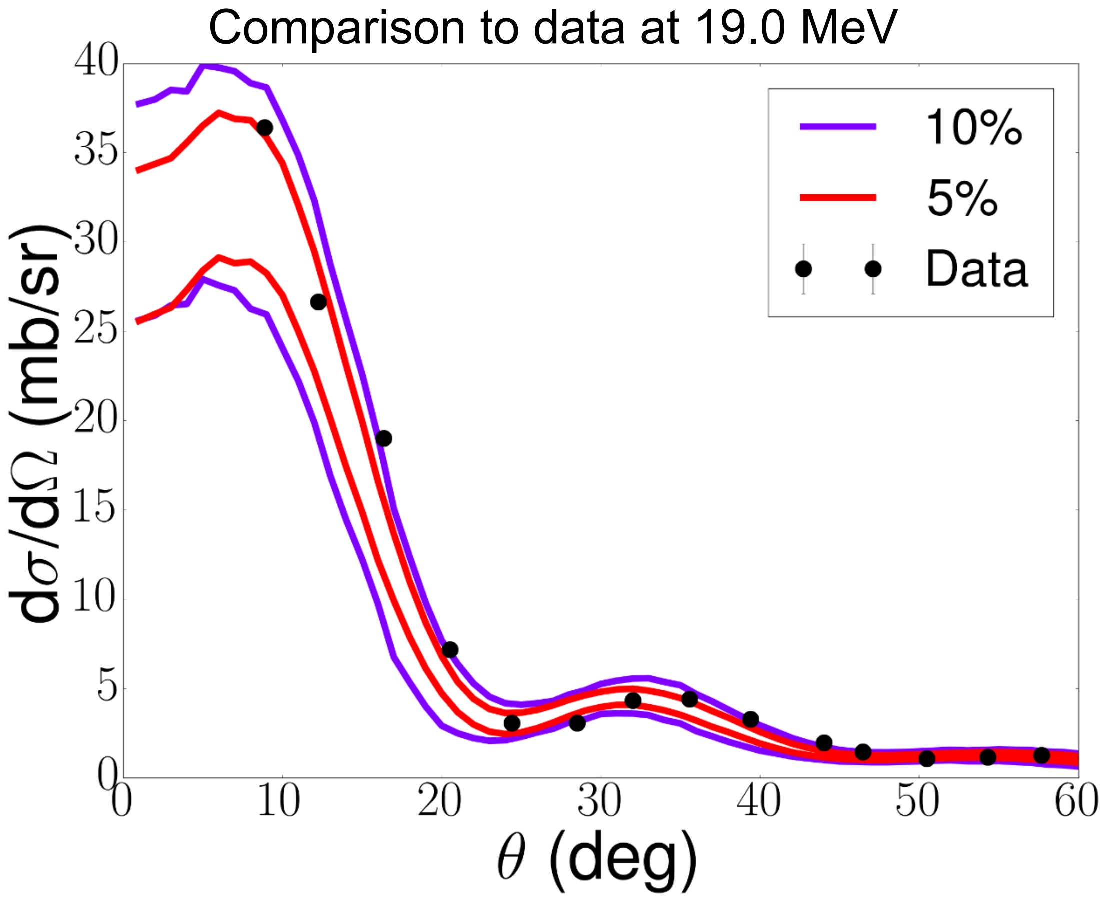


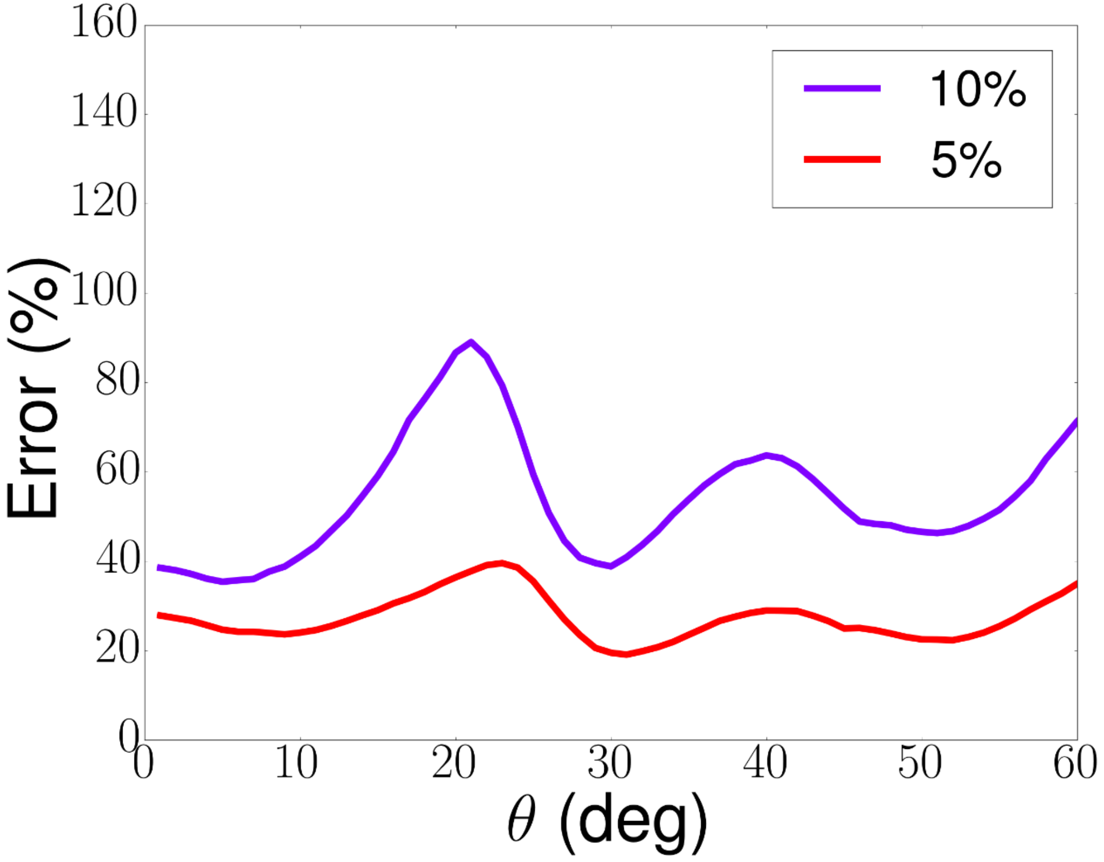


^{48}Ca(p,p) at 25.0 MeV

Data from:
Phys. Rev. C **83** 064605 (2011)
Nucl. Phys. A **188** 103 (1972)
Phys. Rev. C **33** 1624 (1986)

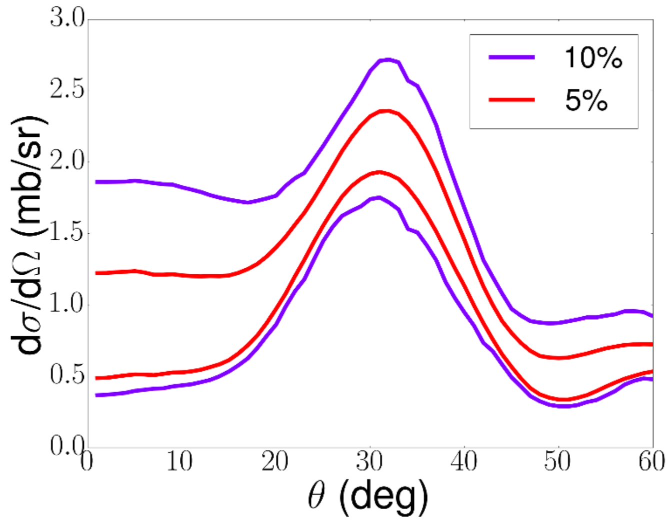
Error Reduction for the Transfer Cross Sections $^{48}Ca(d,p)^{49}Ca(g.s.)$



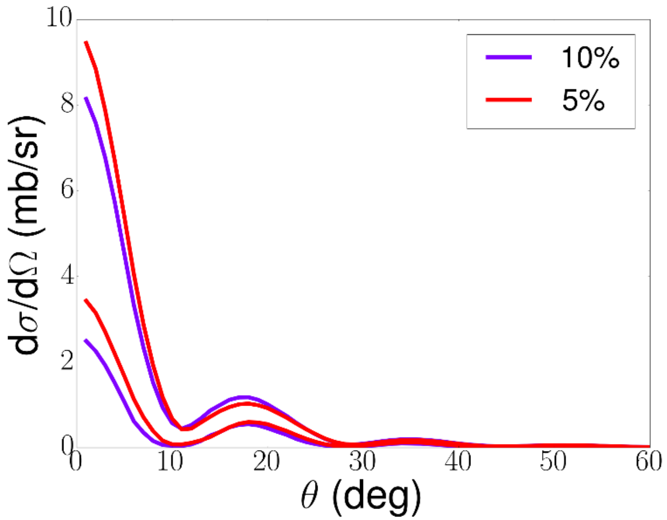


Data extracted from: A.M. Mukhamedzhanov, F.M. Nunes, and P. Mohr, PRC **77** 051601 (2008)

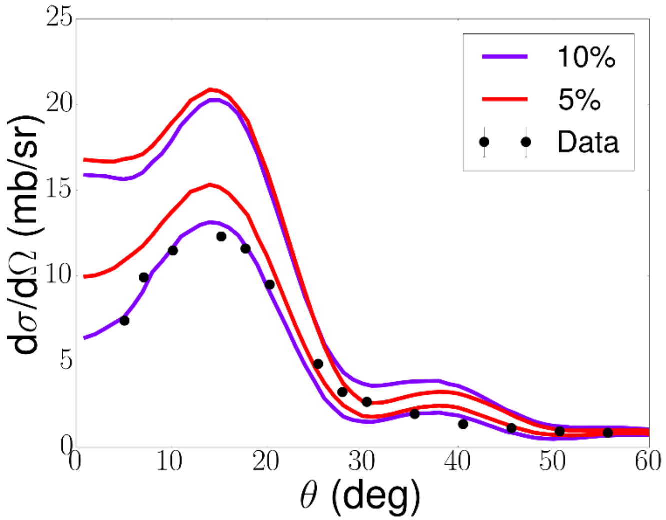
Summary of Results



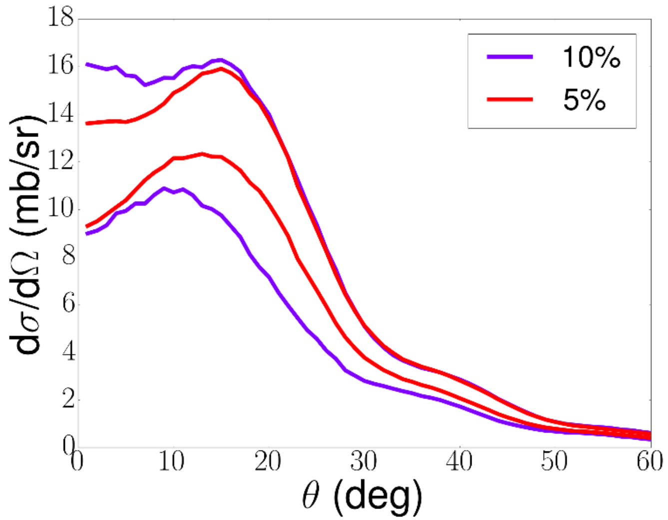
$^{90}Zr(d,n)^{91}Nb$ @ 20.0 MeV



$^{116}Sn(d,p)^{117}Sn$ @ 44.0 MeV

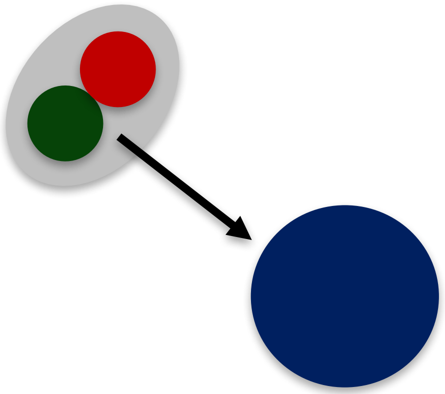


$^{90}Zr(d,p)^{91}Zr$ @ 22.0 MeV



$^{208}Pb(d,p)^{209}Pb$ @ 32.0 MeV

Distorted Wave Born Approximation (DWBA)



ADWA

$$\Psi^{\rm ad}(\vec{r},\vec{R}) = \phi_0(\vec{r})\chi_0^{\rm ad}(\vec{R}) + \sum_{i>0} \phi \cdots {}^{\rm ad}(\vec{R})$$

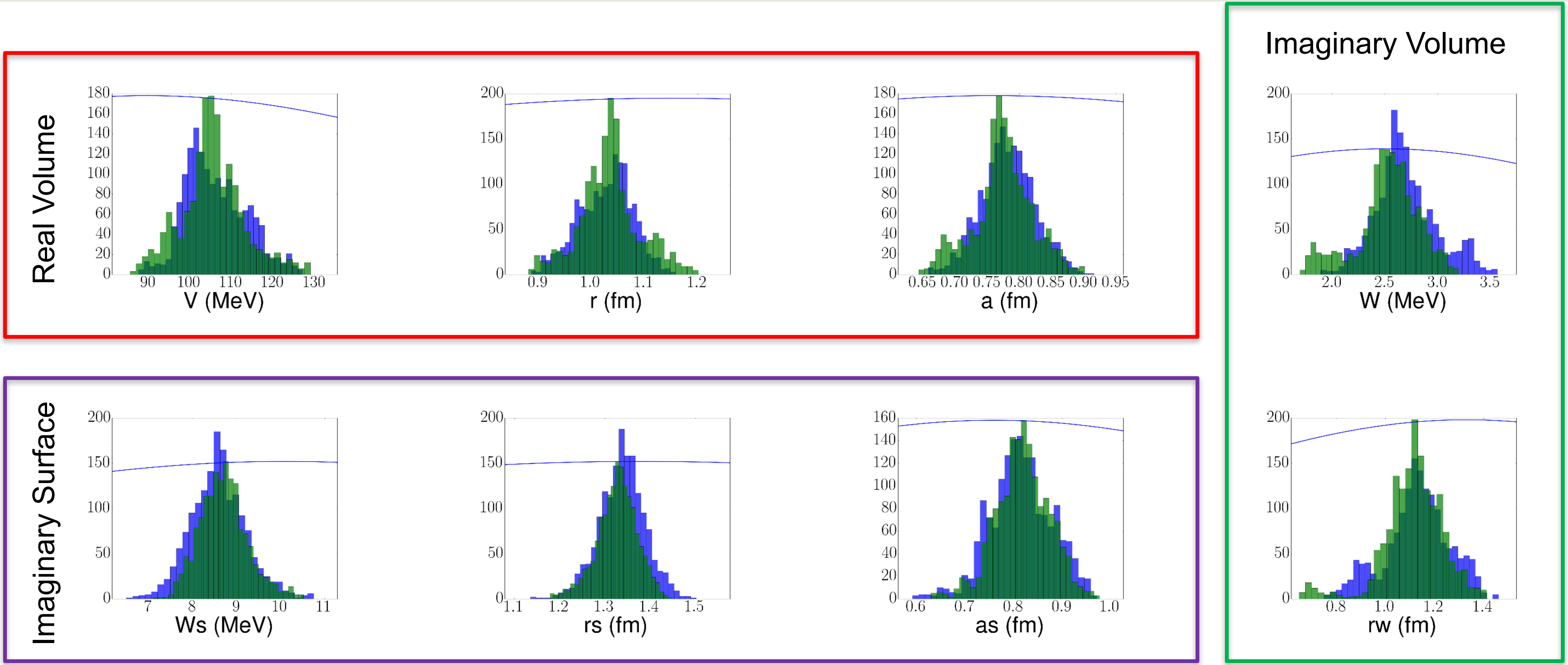
DWBA

$$\Psi^{\rm DWBA}(\vec{r},\vec{R}) = \phi_d(\vec{r})\chi_{dA}(\vec{R})$$

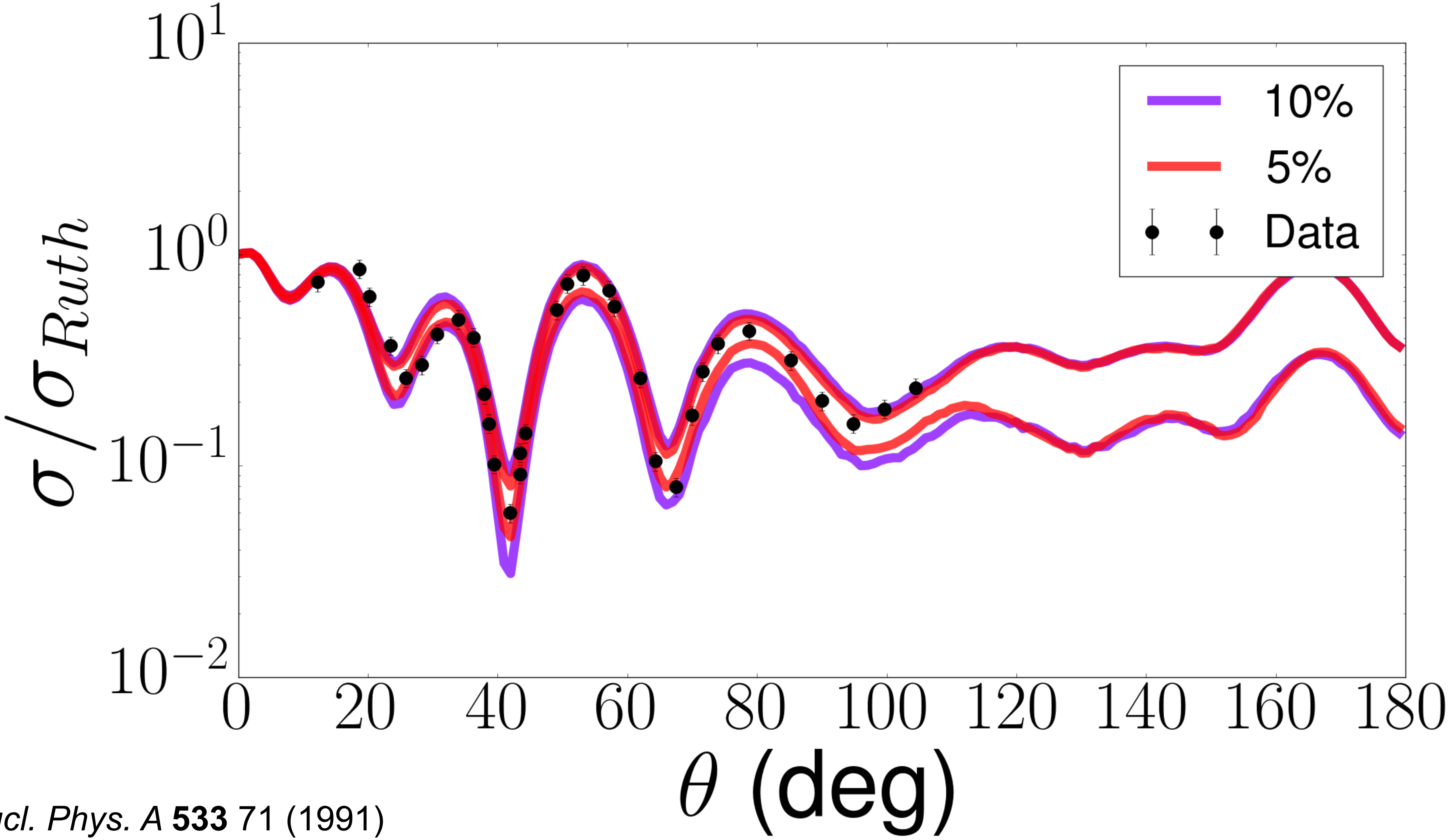
DWBA does not explicitly take into account the breakup of the deuteron and is generally considered a more simplistic theory

I.J. Thompson and F.M. Nunes, *Nuclear Reactions for Astrophysics*, (Cambridge University Press, Cambridge, 2009)

Posterior Calculations (DWBA)
^{48}Ca(d,d) at 23.3 MeV

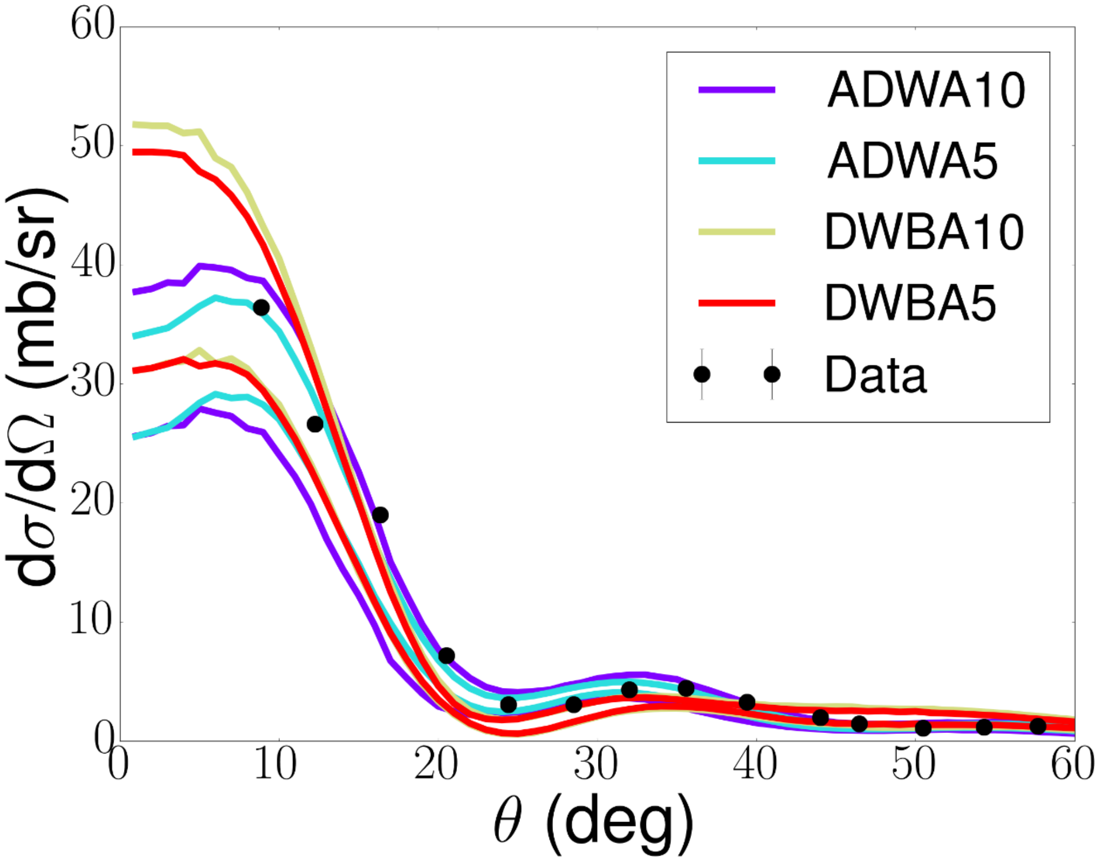


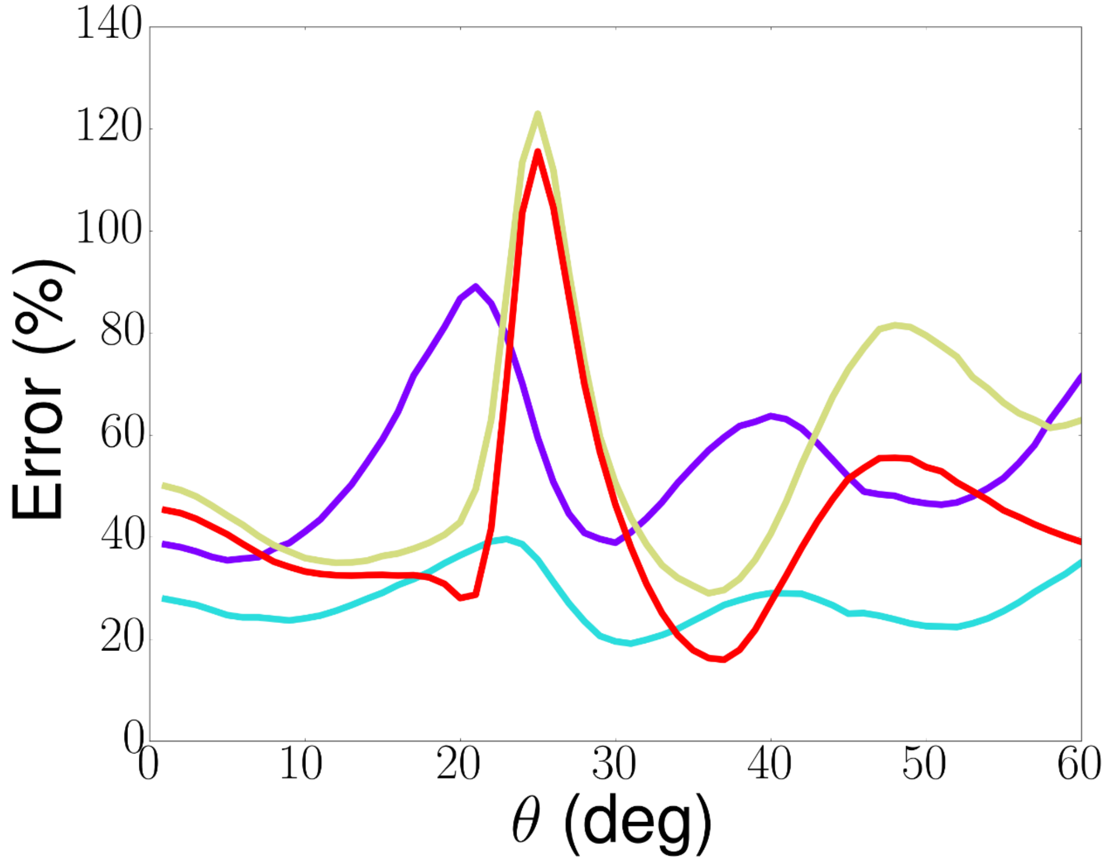
Angular Distributions (DWBA)
$^{48}Ca(d,d)$ at 23.3 MeV



Data from: *Nucl. Phys. A* **533** 71 (1991)

Comparison Between ADWA and DWBA
$^{48}Ca(d,p)^{49}Ca(g.s.)$





Data extracted from: A.M. Mukhamedzhanov, F.M. Nunes, and P. Mohr, PRC **77** 051601 (2008)

Complete Summary of Results

- Studied five transfer reactions with ADWA and DWBA using 10% and 5% experimental errors
- A reduction in the experimental error on the elastic scattering cross section reduces the width of the corresponding transfer cross section prediction
- The theoretical errors are generally reduced when ADWA is used compared to DWBA

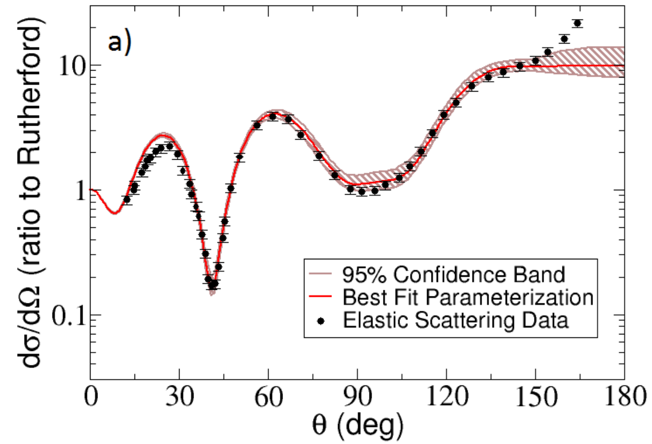
System	Theory	Angle	Peak*	Error_{95}	Error_{68}
$^{48}Ca(d,p)$	ADWA10	6	34.09	35.76	16.47
$^{48}Ca(d,p)$	ADWA5	6	33.38	24.24	11.53
$^{48}Ca(d,p)$	DWBA10	3	41.56	47.93	22.57
$^{48}Ca(d,p)$	DWBA5	4	40.73	42.03	22.36
$^{90}Zr(d,n)$	ADWA10	31	2.16	44.44	17.59
$^{90}Zr(d,n)$	ADWA5	31	2.13	20.19	9.91
$^{90}Zr(d,n)$	DWBA10	31	3.04	38.82	21.52
$^{90}Zr(d,n)$	DWBA5	30	3.15	26.35	13.29
$^{90}Zr(d,p)$	ADWA10	14	16.63	47.62	21.95
$^{90}Zr(d,p)$	ADWA5	14	17.94	30.88	14.99
$^{90}Zr(d,p)$	DWBA10	16	17.09	58.86	29.02
$^{90}Zr(d,p)$	DWBA5	16	17.41	30.61	14.26
$^{116}Sn(d,p)$	ADWA10	1	4.64	121.77	48.31
$^{116}Sn(d,p)$	ADWA5	1	5.93	101.52	55.12
$^{208}Pb(d,p)$	ADWA10	11	13.32	37.84	18.95
$^{208}Pb(d,p)$	ADWA5	14	13.97	25.48	11.42
$^{208}Pb(d,p)$	DWBA10	9	7.44	72.72	43.84
$^{208}Pb(d,p)$	DWBA5	7	8.38	63.01	30.08

Previous Statistical Study of Uncertainties

Previously used χ^2 minimization methods to create 95% confidence bands around a best fit and prediction

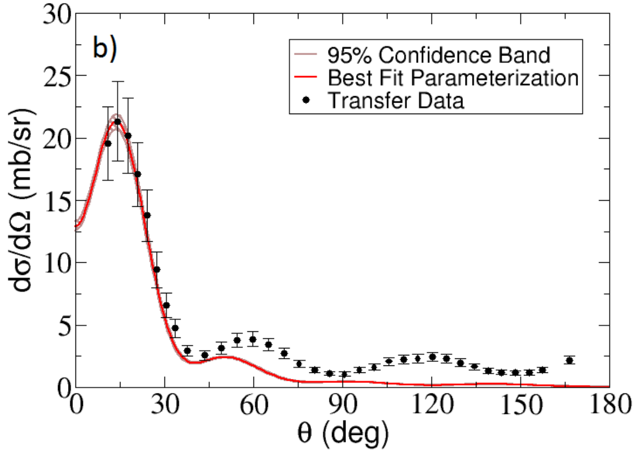
$$\chi^2_{UC}(\mathbf{x}) = \sum_{i=1}^{M} \left(\frac{\sigma^{\text{th}}(\mathbf{x}, \theta_i) - \sigma_i^{\text{exp}}}{\Delta\sigma_i} \right)^2$$

$$\mathcal{N}(\hat{\mathbf{x}}, \mathbb{C}_p) \sim \exp[-\frac{1}{2}(\mathbf{x} - \hat{\mathbf{x}})^T \mathbb{C}_p (\mathbf{x} - \hat{\mathbf{x}})]$$



$^{12}C(d,d)^{12}C$ @ 12 MeV

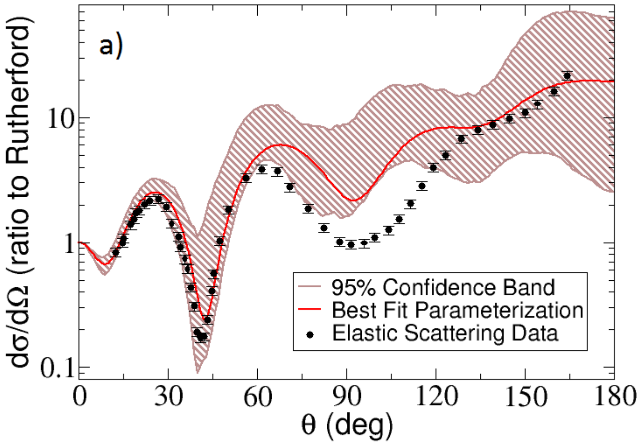
$^{12}C(d,p)^{12}C$ @ 12 MeV



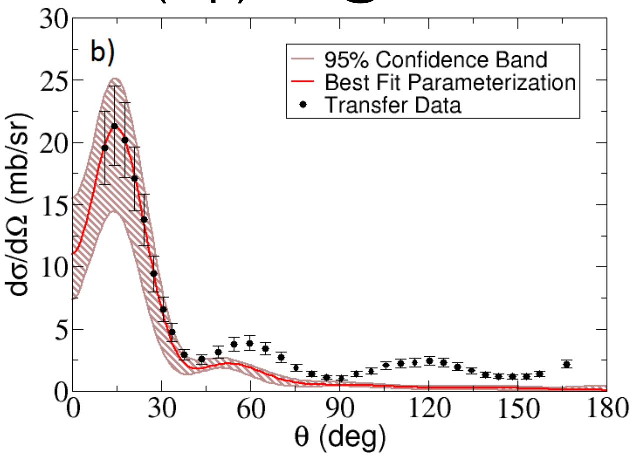
A.E. Lovell, F.M. Nunes, J. Sarich, S.M. Wild, PRC **95** 024611 (2017)

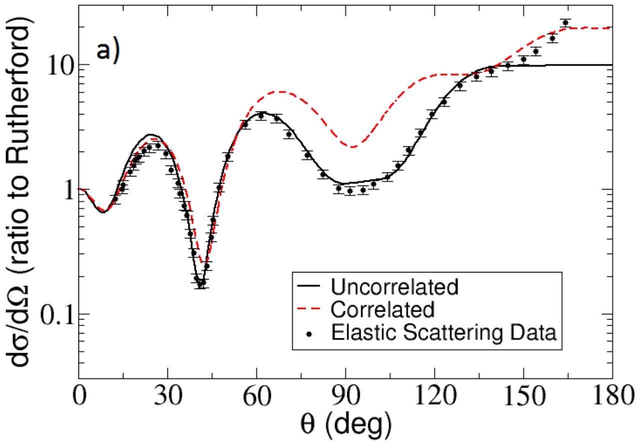
Comparison of Fitting Methods

^{12}C(d,d)^{12}C @ 12 MeV

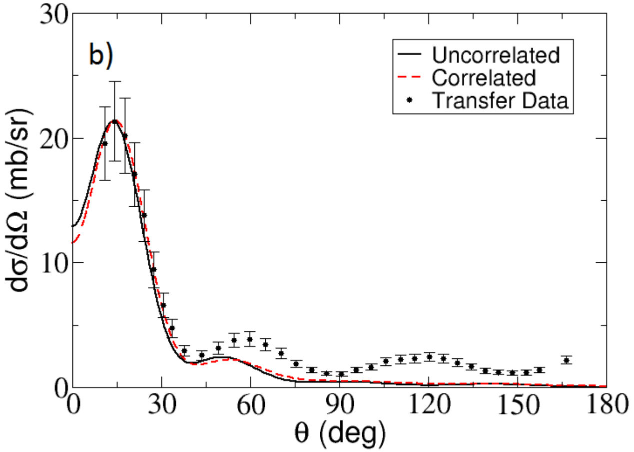


^{12}C(d,p)^{12}C @ 12 MeV





$$\chi^2_C(\hat{\mathbf{x}}) = \sum_{i=1}^{M}\sum_{j=1}^{M} W_{ij}(\sigma^{\rm th}(\mathbf{x},\theta_i) - \sigma_i^{\rm exp})(\sigma^{\rm th}(\mathbf{x},\theta_j) - \sigma_j^{\rm exp})$$



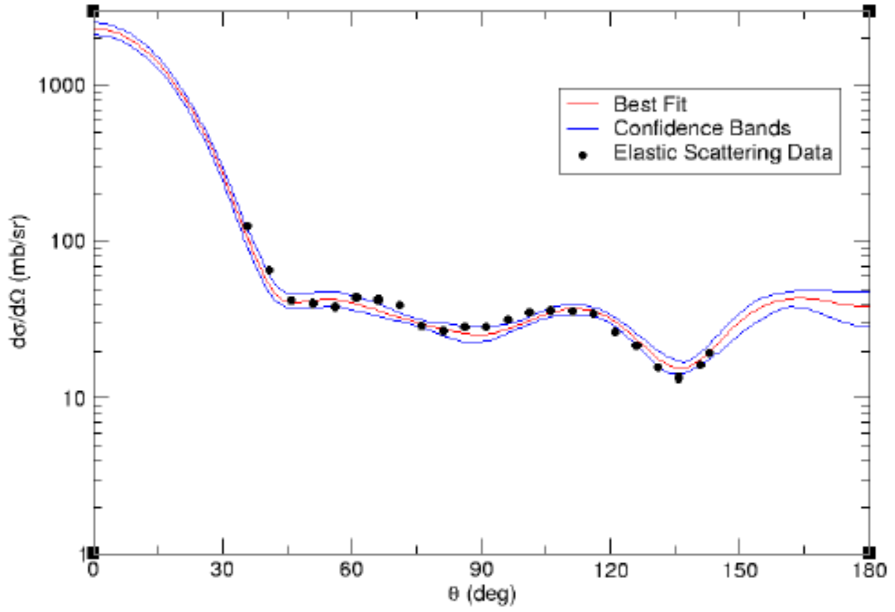
A.E. Lovell, F.M. Nunes, J. Sarich, S.M. Wild, PRC **95** 024611 (2017)

Comparison with Frequentist Methods

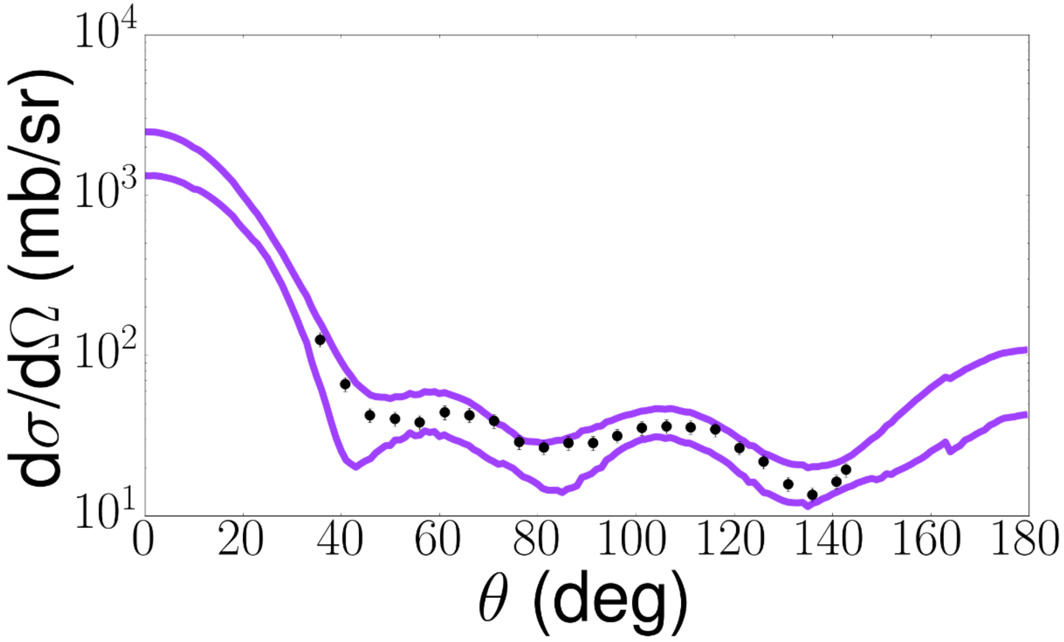
Work done by Garrett King

System	Frequentist	Bayesian
$^{48}Ca(d,p)^{49}Ca$	21.79%	35.76%
$^{90}Zr(d,p)^{91}Zr$	13.29%	47.62%
$^{116}Sn(d,p)^{117}Sn$	68.23%	121.77%
$^{208}Pb(d,p)^{209}Pb$	33.84%	37.84%

Preliminary



$^{48}Ca(n,n)$ @ 12.0 MeV



Summary

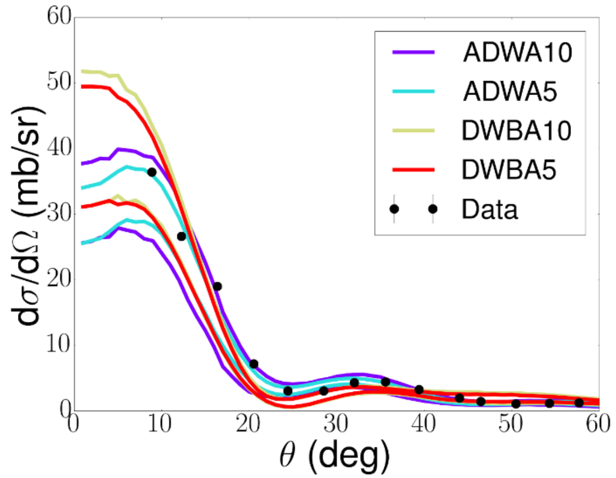
- Uncertainty quantification is being introduced into direct reaction theory
- Bayesian methods have been used to constrain the optical potential parameters for ^{48}Ca-p, ^{48}Ca-n, and ^{48}Ca-d to be introduced into the adiabatic wave approximation (ADWA) and the distorted-wave Born approximation (DWBA)
- Although the elastic scattering is very well constrained, the confidence intervals for transfer predictions are wider
- The reduction of the experimental error bars was studied and does reduce the uncertainty in the resulting cross section – but not proportionally to the reduction in the experimental errors
- We can directly compare ADWA and DWBA in terms of the confidence intervals that are predicted for the ^{48}Ca(d,p)^{49}Ca(g.s.) transfer reaction which is leading to more rigorous model comparison

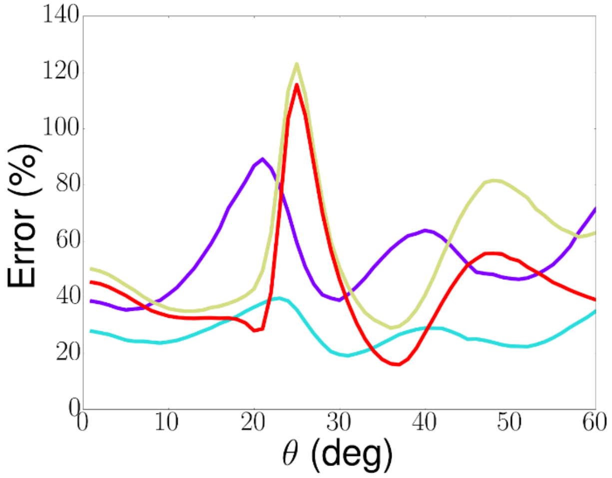
Outlook: Model Uncertainties

$$P(\mathcal{D})$$

Evidence – marginal distribution of the data given the likelihood and the prior

$$P(\mathcal{D}) = \sum P(\mathcal{H})P(\mathcal{D}|\mathcal{H})$$

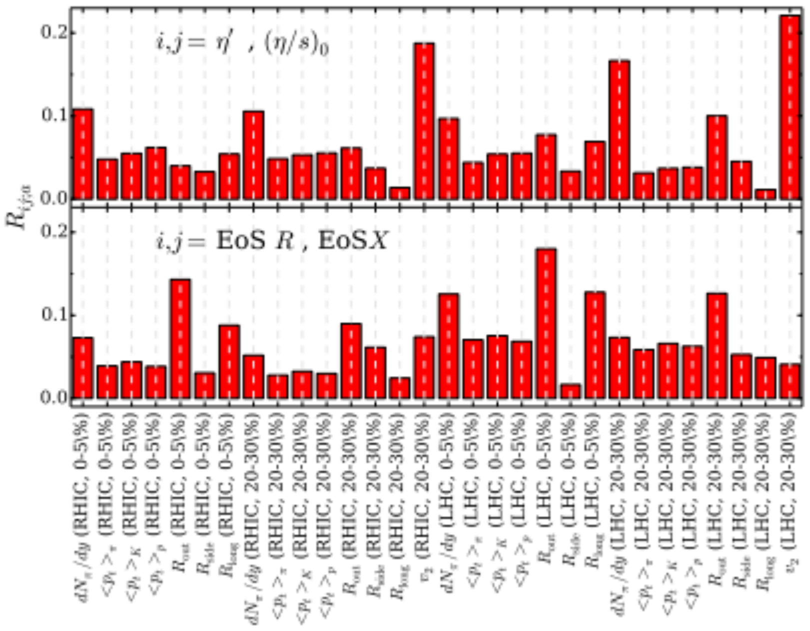




Outlook: Including the Right Information

- We want to understand if the data we are using to constrain the potentials is enough to constrain all of the parameters within our models

- Use Principle Component Analysis (PCA) to study this – understand how much information is actually contained in elastic scattering (do we need total cross sections, radii, other channels, etc.?)



E. Sangaline and S. Pratt,
arXiv:1508.07017v2 [nucl-th] 4 Oct 2015

Acknowledgements

- Filomena Nunes, Garrett King, and the few-body group (NSCL/MSU)
- David Higdon (Virginia Tech)
- Dick Furnstahl (Ohio State University)
- iCER and HPCC (MSU) for computational resources
- DOE Stewardship Science Graduate Fellowship

Thank you!

Any questions?