Uncertainty quantification in reaction theory

Filomena Nunes
Michigan State University

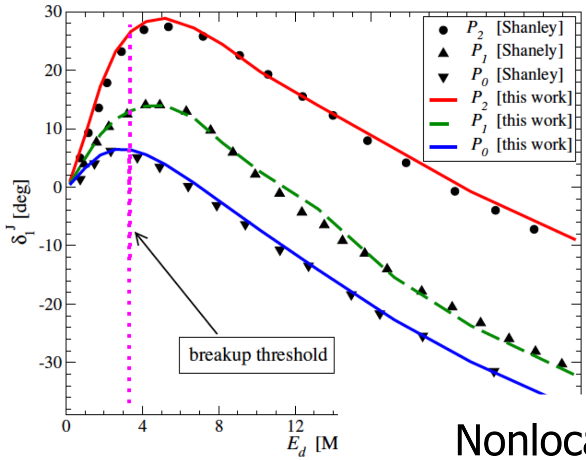
In collaboration with:
Amy Lovell, Garrett King (MSU)
Stephan Wild and Jason Sarich (ANL)

Supported by: NNSA-DOE, NSF

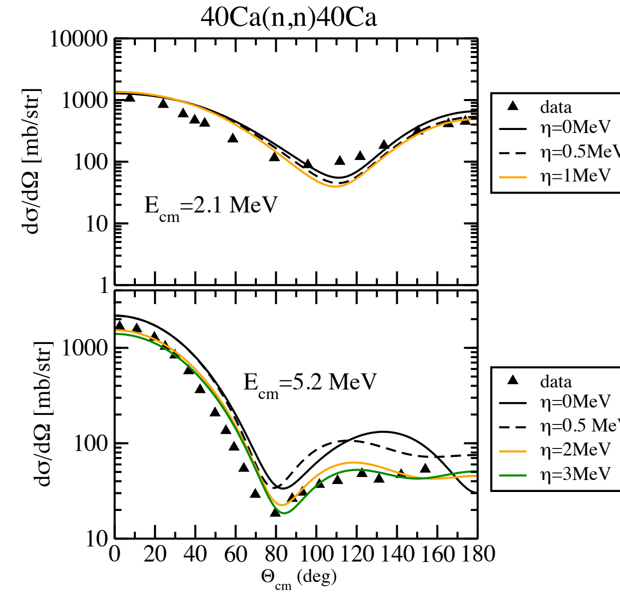
Trento, March 2018

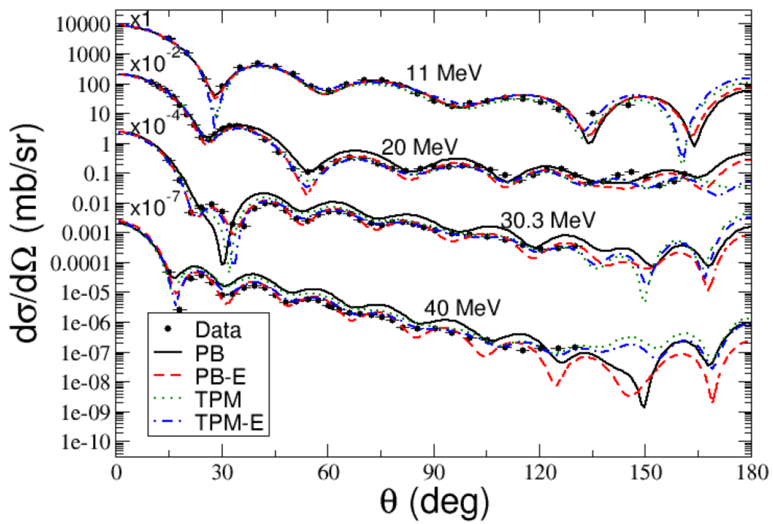
Reaction efforts at MSU

Faddeev in Coulomb basis with separable interactions (Hlophe, Lin, CE, AN, FN)



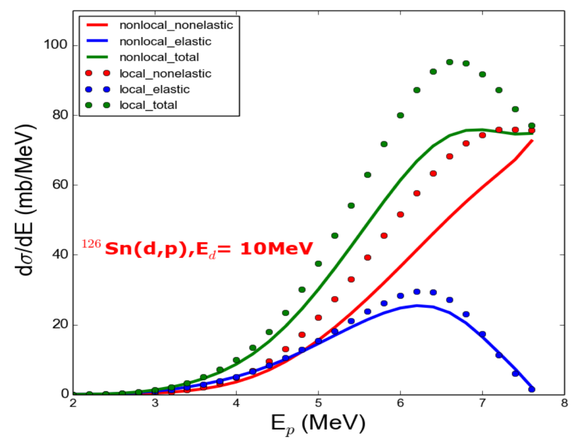
Microscopic optical potential (Rotureau, FN, et al)



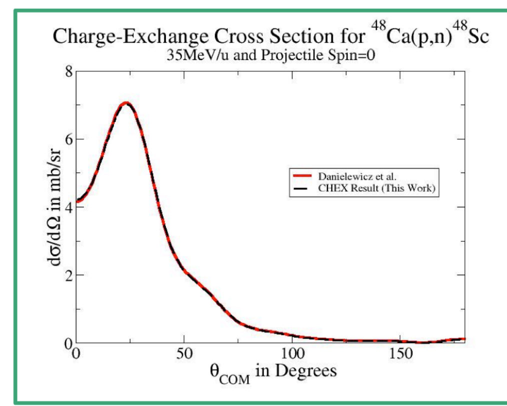


Non-local global nA and pA potential (Bacq, Capel, Jaghoub, Lovell, FN)

Nonlocal effects in (d,p) inclusive (Potel, Li, FN)



Charge-exchange (Poxon-Pearson, Potel, FN)



Uncertainty quantification in reaction theory

Filomena Nunes
Michigan State University

In collaboration with:
Amy Lovell, Garrett King (MSU)
Stephan Wild and Jason Sarich (ANL)

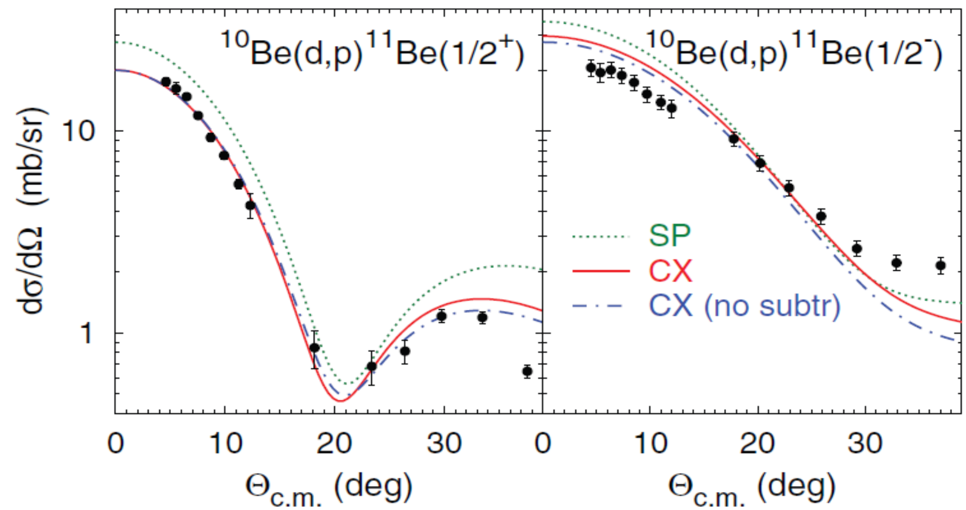
Supported by: NNSA-DOE, NSF

Trento, March 2018

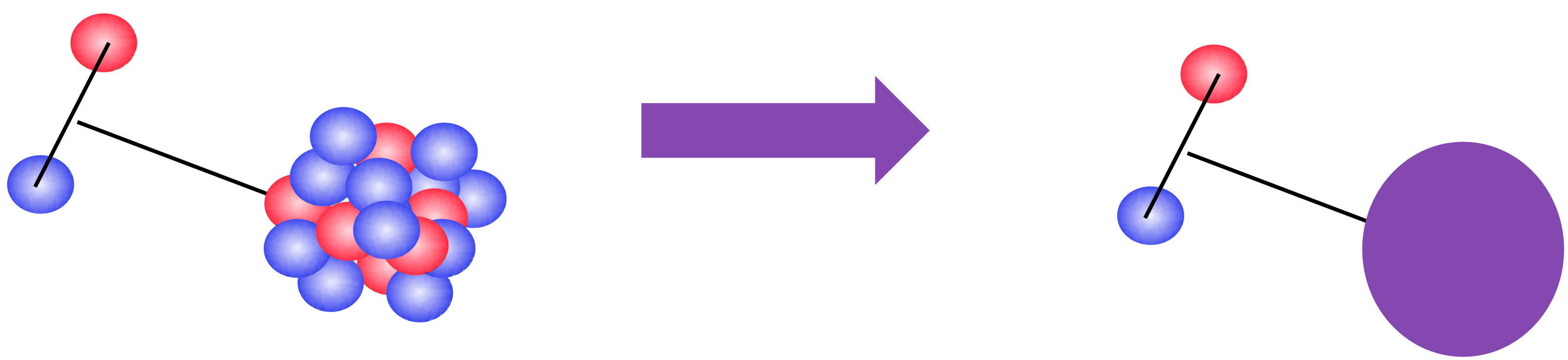
What is the nuclear physics problem: how certain are our reaction predictions?

A(d,p)B

Deuteron induced reactions typically treated as a three-body problem



Deltuva, PRC91, 024607 (2015)



What is the UQ problem:

We develop a hypothesis (model)

We confront it with reality (data)

How good is the model?

What is the UQ problem:

We develop a hypothesis (model)

DWBA or ADWA

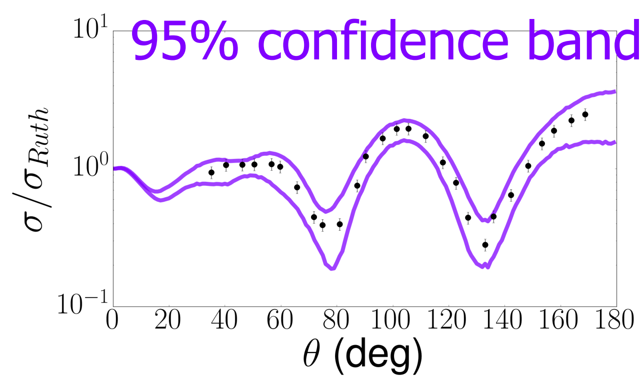
We confront it with reality (data)

Introducing a function, e.g.

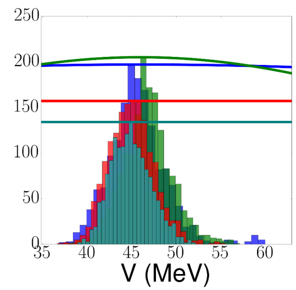
$$\chi^2 = \sum_{i=1}^{n} \left(\frac{m(\mathbf{x};\theta_i) - d_i}{\sigma_i} \right)^2$$

How good is the model?

95% confidence bands



Constrains on the model



What is the model?

DWBA

Exact T-matrix for A(d,p)B in POST from:

$$T_{post} = < \phi_{nA}\, \chi_{pB}^{(-)} \mid \Delta V_f \mid \Psi_1^{(+)}(\vec{r}_1, \vec{R}_1) >$$

deuteron elastic component

Take first term of Born series: $\Psi_1^{(+)}(\vec{r}_1, \vec{R}_1) \rightarrow \phi_{np}\, \chi_{dA}$

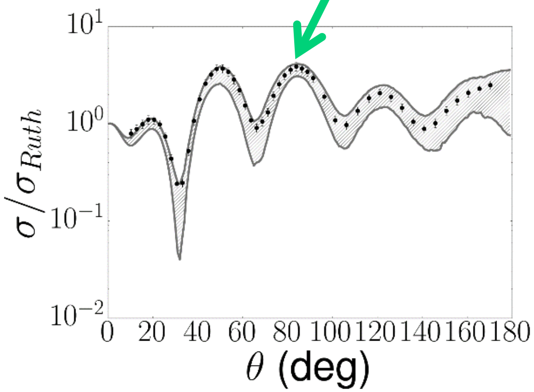
$$T_{post}^{DWBA} = < \phi_{nA}\, \chi_{pB}^{(-)} \mid \Delta V_f \mid \phi_{np}\, \chi_{dA} >$$

What is the input from reality?

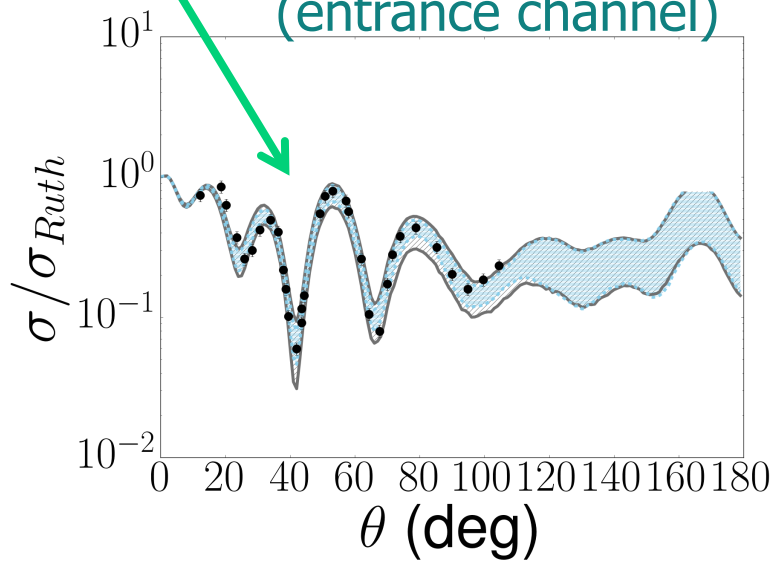
DWBA

$$T_{post}^{DWBA} =< \phi_{nA}\, \chi_{pB}^{(-)} \mid \Delta V_f \mid \phi_{np}\, \chi_{dA} >$$

proton elastic data
(exit channel)



deuteron elastic data
(entrance channel)



What is the model?

ADWA

Johnson and Tandy, NPA1974

Exact T-matrix for A(d,p)B in POST from:

$$T_{post} =< \phi_{nA}\, \chi^{(-)}_{pB} \mid \Delta V_f \mid \Psi^{(+)}_1(\vec{r}_1, \vec{R}_1) >$$

finite range adiabatic approximation

Adiabatic wave approximation:

3B wave function expanded in Weinberg states

$$\Psi^{\text{exact}} = \sum_{i=0}^{\infty} \phi_i(\vec{r})\chi_i(\vec{R})$$

$$(T + \lambda_i V_{np} - \epsilon_d)\phi_i = 0$$

$$U_{ij}(\vec{R}) = -\langle \phi_i | V_{np}(U_{nA} + U_{pA}) | \phi_j \rangle$$

Typically, only keep the first Weinberg State

$$\Psi^{ad} \approx \phi_0(\vec{r})\chi_0(\vec{R})$$

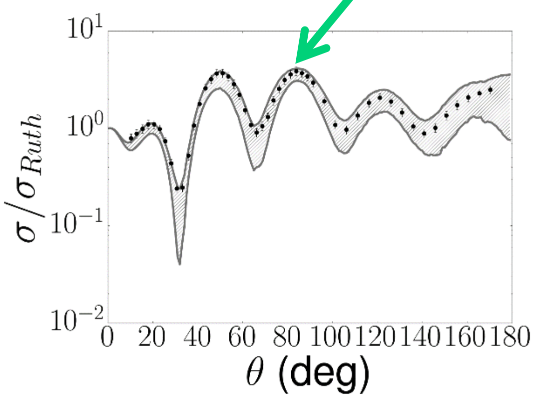
What is the input from reality?

AWBA

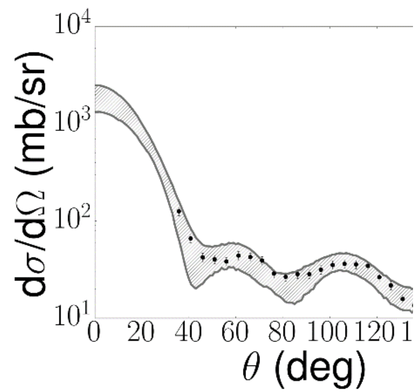
$$T^{(d,p)} = \langle \phi_{An} \chi_p | V_{np} | \phi_d \chi_d^{ad} \rangle$$

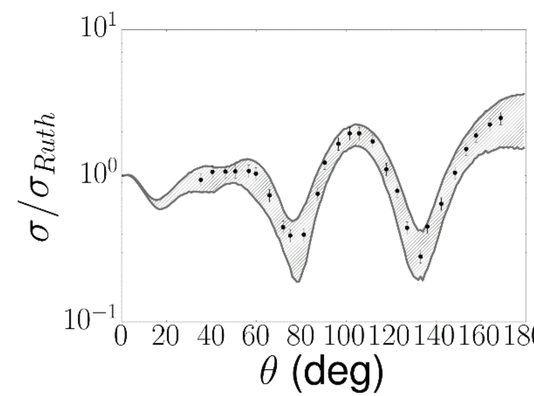
$$U_{ij}(\vec{R}) = -\langle \phi_i | V_{np} (U_{nA} + U_{pA}) | \phi_j \rangle$$

proton elastic data
(exit channel)



neutron and proton elastic data
(entrance channel)





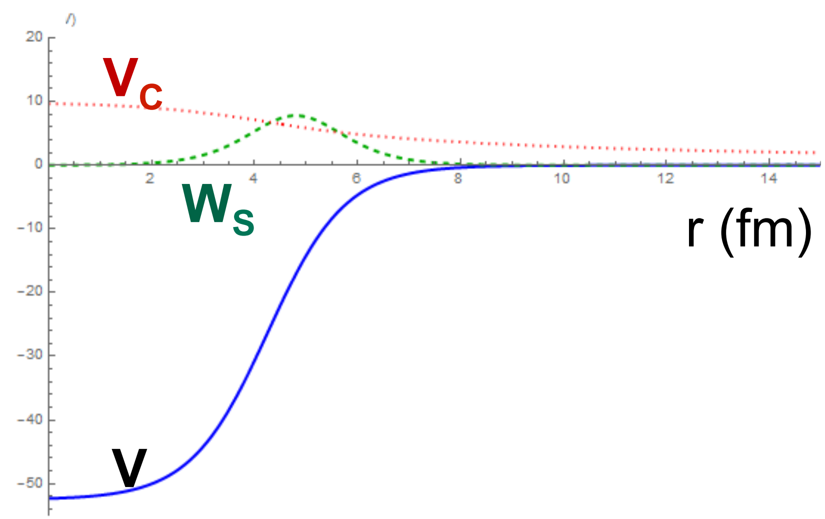
What are the parameters of the model?

Optical potentials (assumed local to reduce computational time)

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

Parameters:

- Volume real V r a
- Volume imaginary W r_W a_W
- Surface imaginary V_s r_s a_s
- Spin-orbit real V_s r_s a_s
- ~~Spin-orbit imaginary V_s r_s a_s~~
- Coulomb r_c



Outline

1. Using uncorrelated chi2 function
2. Using correlated chi2 function
3. Using Bayes' Theorem
4. Conclusions
5. Outlook

Standard Chi2 minimization

- Have n observable pairs (d_i,θ_i) that are linked by a true function, $\mu(\theta_i)$, such that: $d_i = \mu(\theta_i) + \epsilon_i$

$$[d_1, ..., d_n]^T \sim \mathcal{N}(\mu, \Sigma) \qquad \epsilon_i \sim \mathcal{N}(0, \sigma_i^2)$$

- In not knowing the true function, we create a model, m(**x**,θ_i), to describe the data

$$d_i = m(\mathbf{x}, \theta_i) + \epsilon_i$$

- In fitting the model to the observables, the goal is to minimize the residuals

- For uncorrelated observables

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{m(\mathbf{x}; \theta_i) - d_i}{\sigma_i} \right)^2$$

Minimizing the residuals

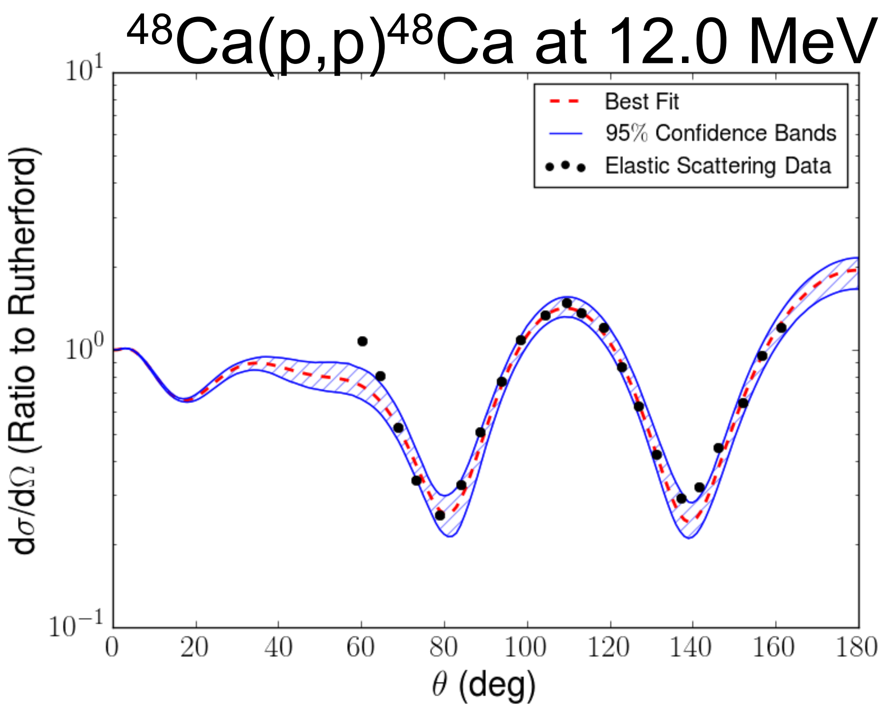
$$[m(\hat{\mathbf{x}}; \theta_1) - d_1, ..., m(\mathbf{x}; \theta_n) - d_n]^T \sim \mathcal{N}(0, \Sigma)$$

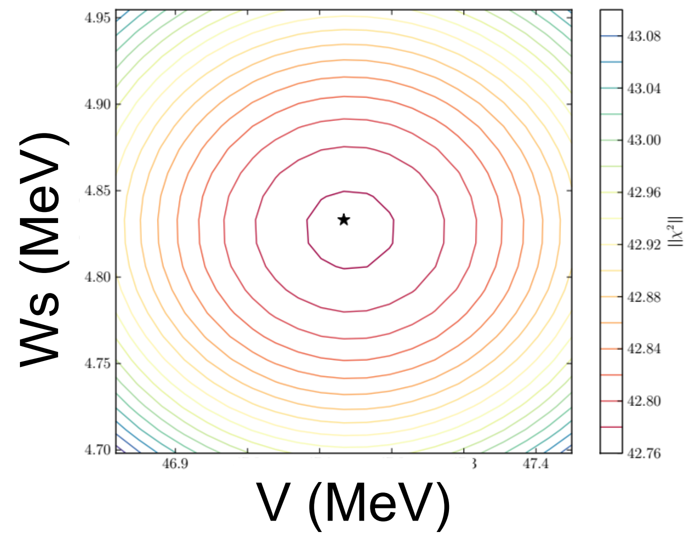
$\hat{\mathbf{x}}$ → Best fit set of parameters

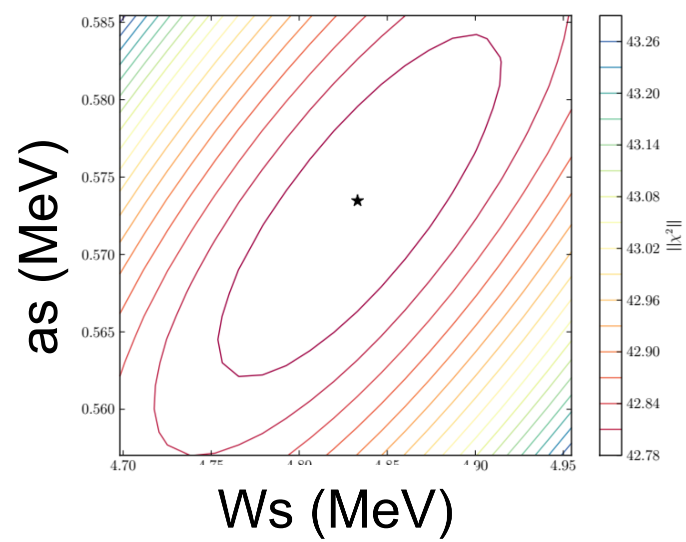
- Pull 200 sets from this distribution and run them through the model

- Create 95% confidence bands by removing the top 2.5% and bottom 2.5% of the calculations at each angle

Standard Chi2 minimization

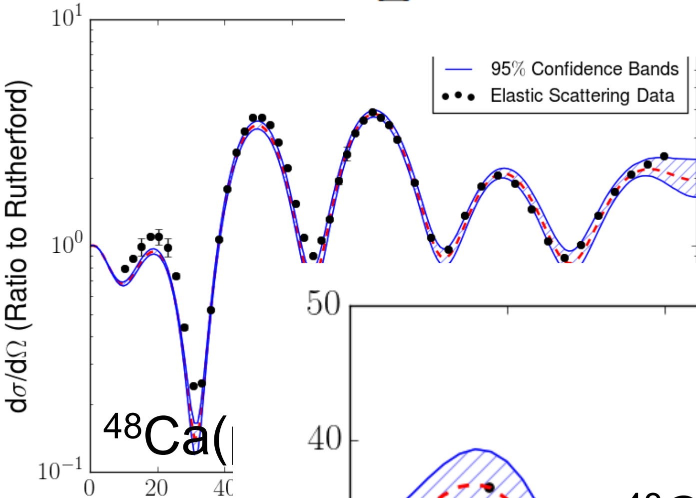


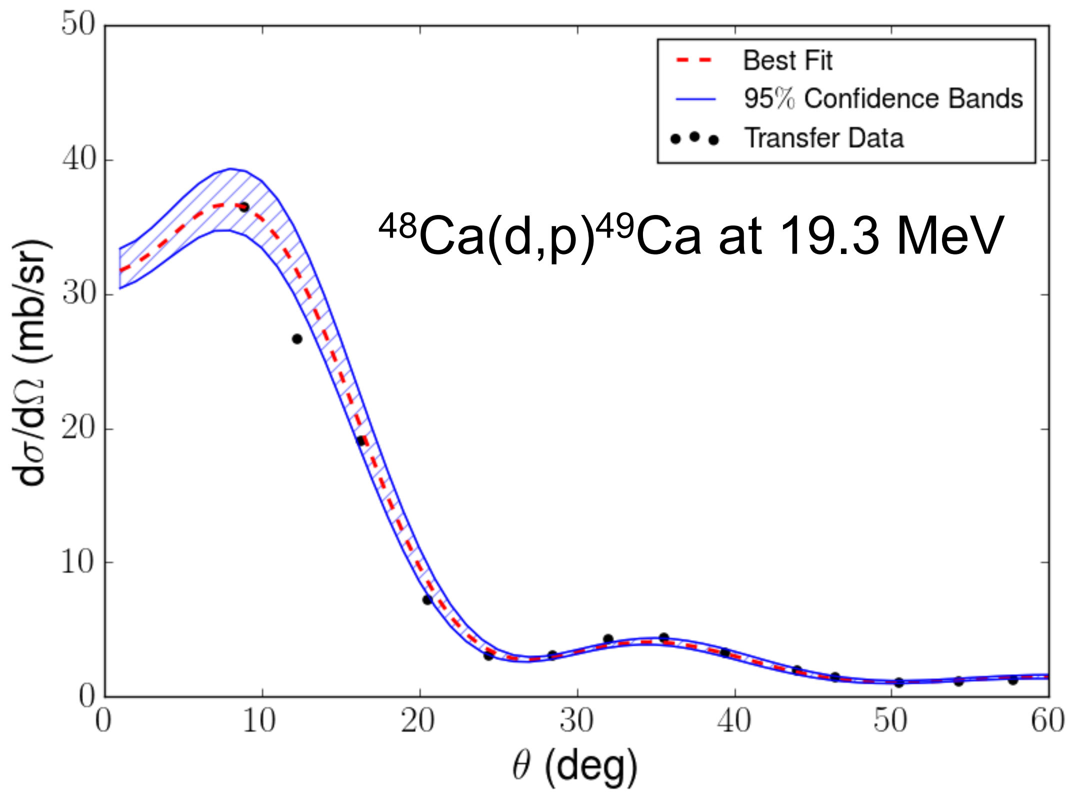


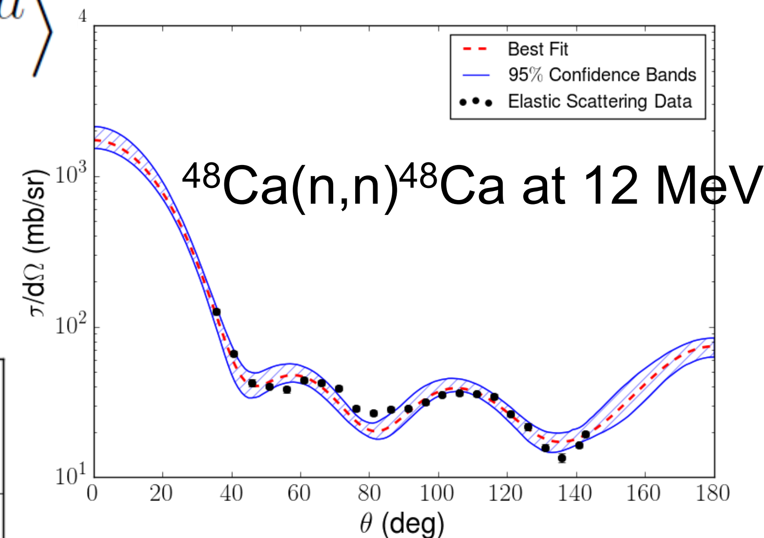


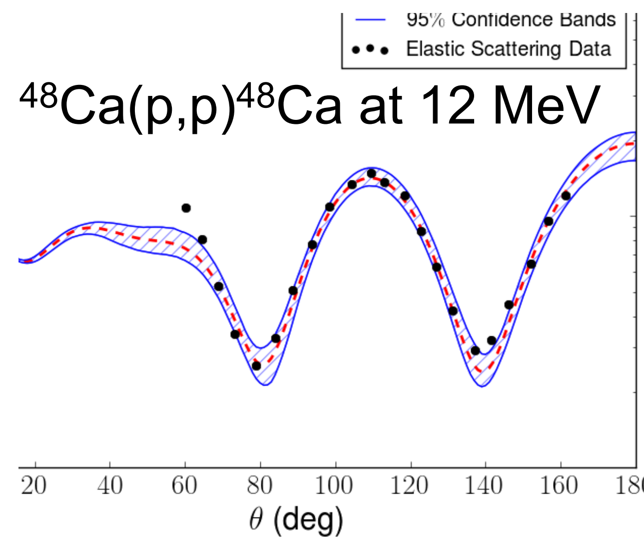
Standard Chi2 minimization

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









Chi2 minimization

Previously: Uncorrelated Model

- Data and residuals are normally distributed

$$[d_1, ..., d_p]^T \sim \mathcal{N}(\mu, \Sigma)$$

$$[m(\mathbf{x}; \theta_1) - d_1, ..., m(\mathbf{x}; \theta_p) - d_p]^T \sim \mathcal{N}(0, \Sigma)$$

- With covariance matrix

$$\Sigma_{ii} = \sigma_i^2$$

- Leads to the minimization function

$$\chi^2 = \sum_{i=1}^{n} \left(\frac{m(\mathbf{x}; \theta_i) - d_i}{\sigma_i} \right)^2$$

Instead: For a Correlated Model

- Model is also normally distributed

$$[m(\mathbf{x}; \theta_1), ..., m(\mathbf{x}; \theta_p)]^T \sim \mathcal{N}(\mu, \mathbb{C}_m)$$

- Residuals then have the distribution

$$[m(\mathbf{x}; \theta_1) - d_1, ..., m(\mathbf{x}; \theta_p) - d_p]^T \sim \mathcal{N}(0, \mathbb{C}_m + \Sigma)$$

- With covariance matrix

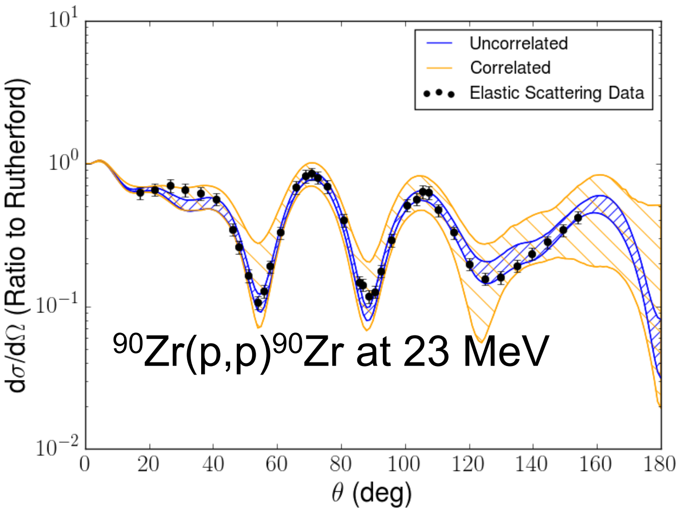
$$\mathbb{C}_m + \Sigma$$

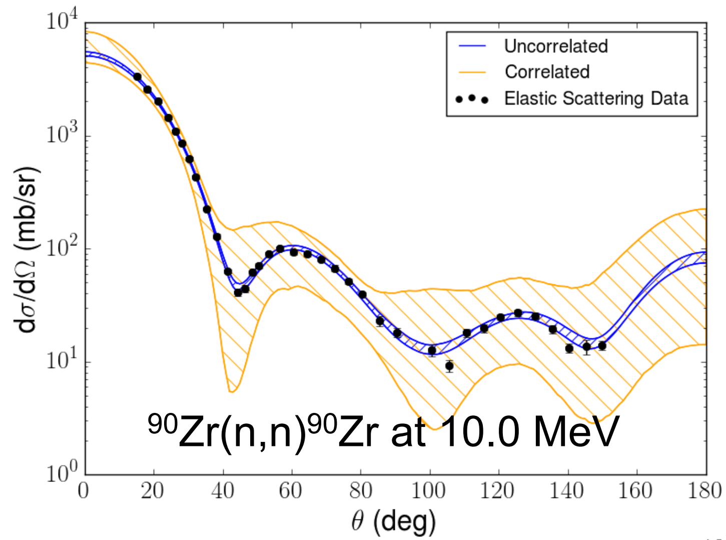
- Leads to the minimization function

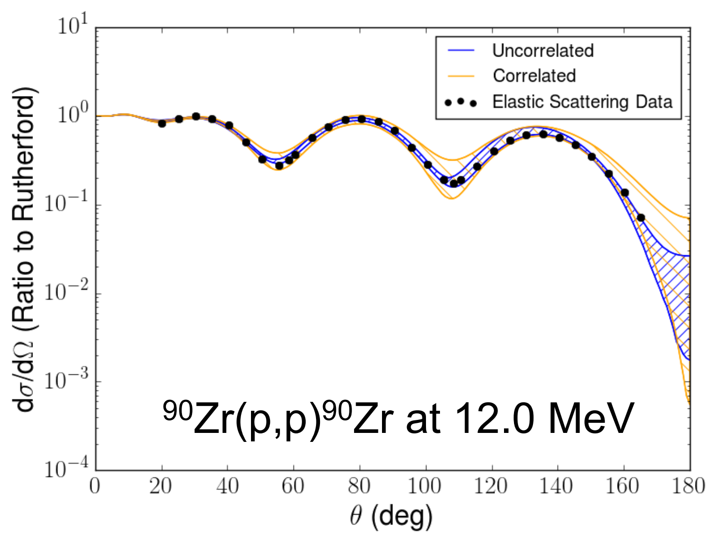
$$\chi^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (m(\mathbf{x}; \theta_i) - d_i)(m(\mathbf{x}; \theta_j) - d_j)$$

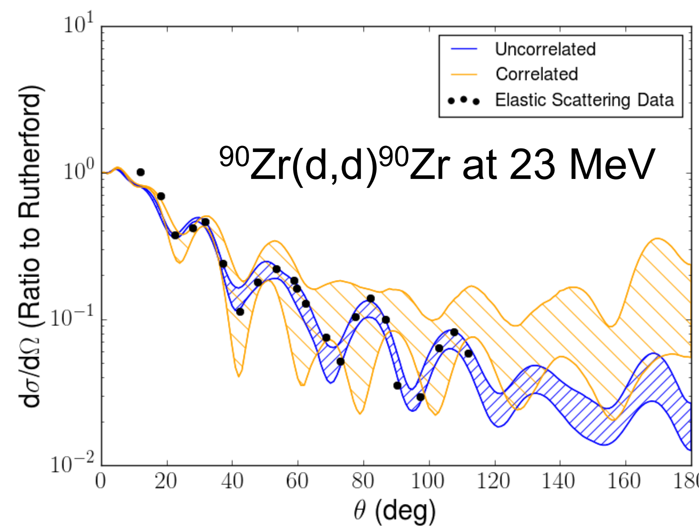
$$W = (\mathbb{C}_m + \Sigma)^{-1}$$

Chi2 minimization: elastic scattering

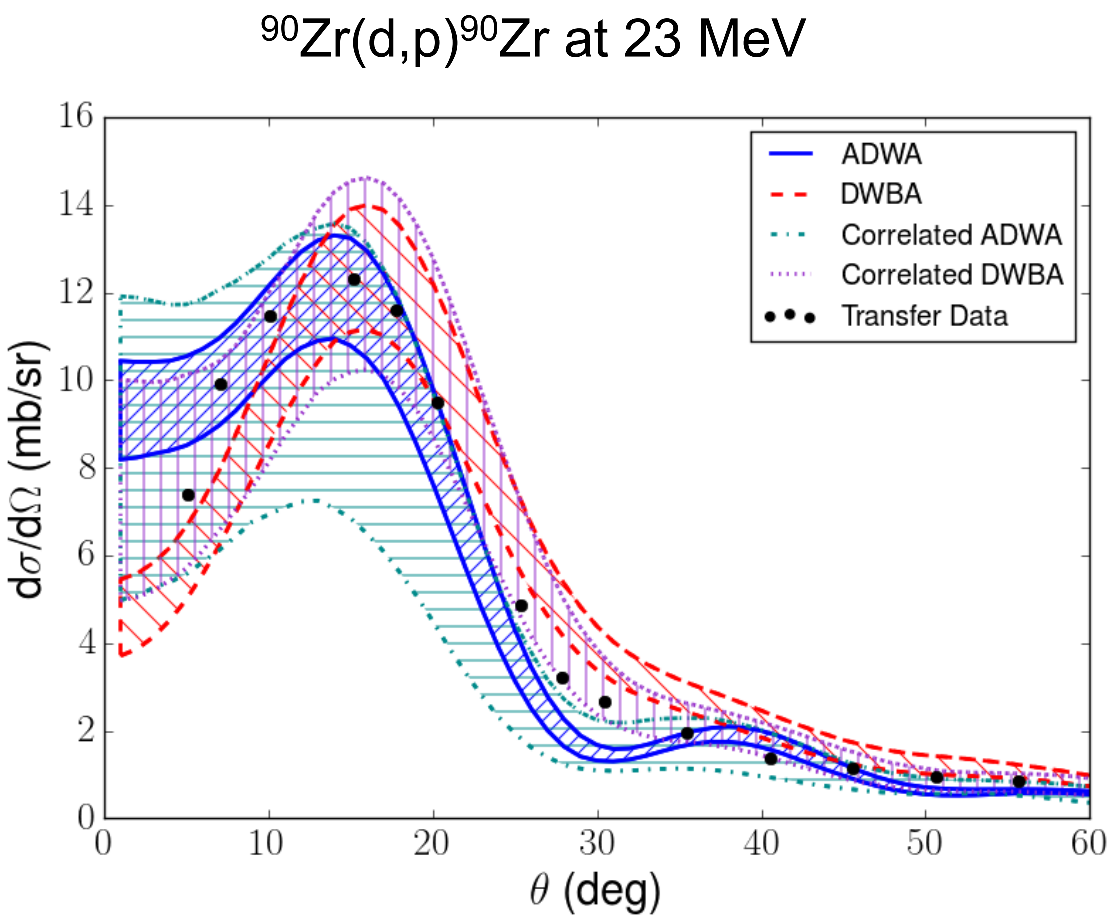








Chi2 minimization: transfer predictions



Chi2 minimization: systematics

Reaction	E (MeV)	Width(DWBA) %	Width(ADWA) %
^{48}Ca(d,p)	19.3	8.2571	11.7164
^{90}Zr(d,p)	22.7	22.94803	19.00016
^{90}Zr(d,n)	19.018	22.22602	11.84450
^{116}Sn(d,p)	46.0	33.68678	9.692527
^{208}Pb(d,p)	32.9	36.5096	24.00519

Limitations of the frequentist approach

Philosophical aspects:

- Probability as frequency: number of events over a total number of trails
- A 95% confidence band means that when repeating the measurement many times, 95% of the times the data should fall within the band.
- There is no way to include UQ on events that cannot be repeated (e.g. how likely is it that I will be run over by a car walking back to trento?).

Practical aspects:

- Problem with local minima versus the global minimum
- Inclusion of prior knowledge comes through ranges allowed for parameters – potential for introducing biases
- What is the correct Chi2 function that includes the correct correlations in the theoretical model?

Comparing frequentist and Bayesian

- Probability as frequency
- A 95% confidence band means that when repeating the measurement many times, 95% of the times the data should fall within the band.

Practical aspects:

- local minima
- ranges allowed for parameters – potential for introducing biases
- correlations in the theoretical model?

- Probability as degree of belief
  - Posterior distribution updates our degree of belief on the model, in light of the data
- A 95% confidence band means, given the data, what are the parameter ranges of the model for a 95% degree of belief.

Practical aspects:

- Markov Chain Monte Carlo (MCMC) spans full space and is fully automated
- Inclusion of prior (no biases)
- Correlations automatically included
- Computationally more expensive

Bayes' theorem

P(green,red)= 5/9 x 4/9

P(red,green)= 4/9 x 5/9

P(green,red)=P(red,green)

Bayesian statistics

Thomas Bayes (1701–1761)

Bayes' Theorem

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

Posterior – probability that the model/parameters are correct after seeing the data

Prior – what is known about the model/ parameters before seeing the data

Likelihood – how well the model/parameters describe the data

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

Markov Chain Monte Carlo (MCMC)

$$p(H_i)p(D|H_i)$$

Randomly choose new parameters

$$p(H_f)p(D|H_f)$$

$$R < \frac{p(H_f)p(D|H_f)}{p(H_i)p(D|H_i)}$$

Bayesian: prior dependence

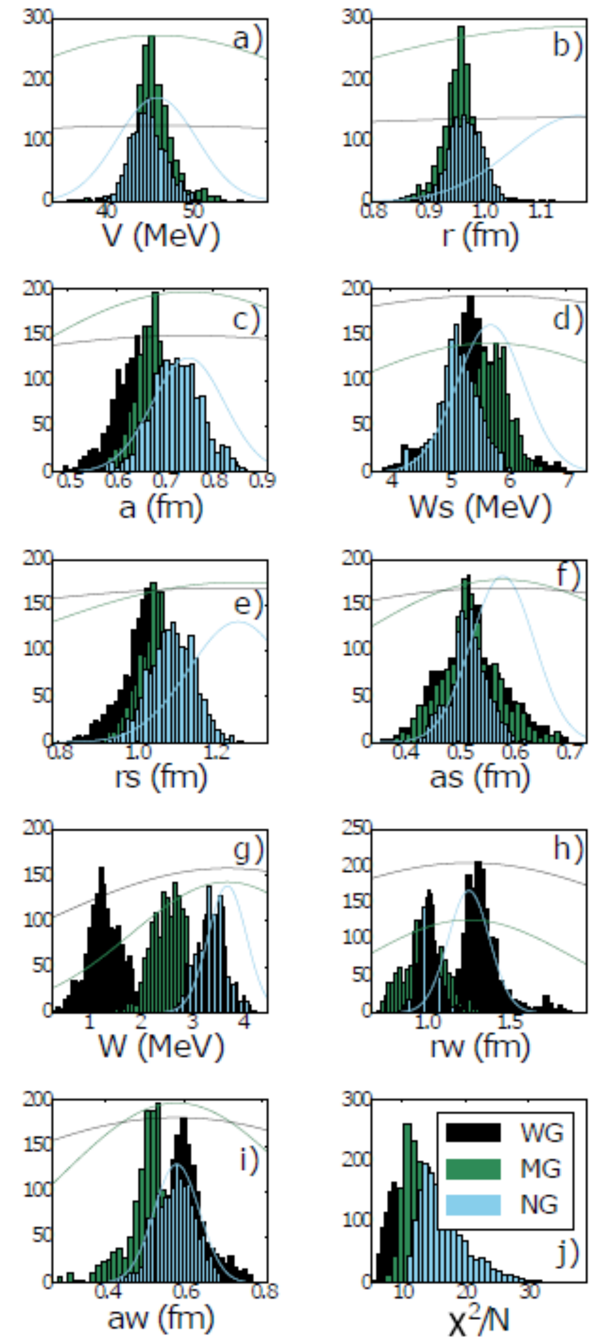
$$p(H) \propto \prod_{i=1}^{N_p} \exp\left[\frac{(x^i - x_0^i)^2}{(x_0^i)^2}\right]$$

Types of Priors:

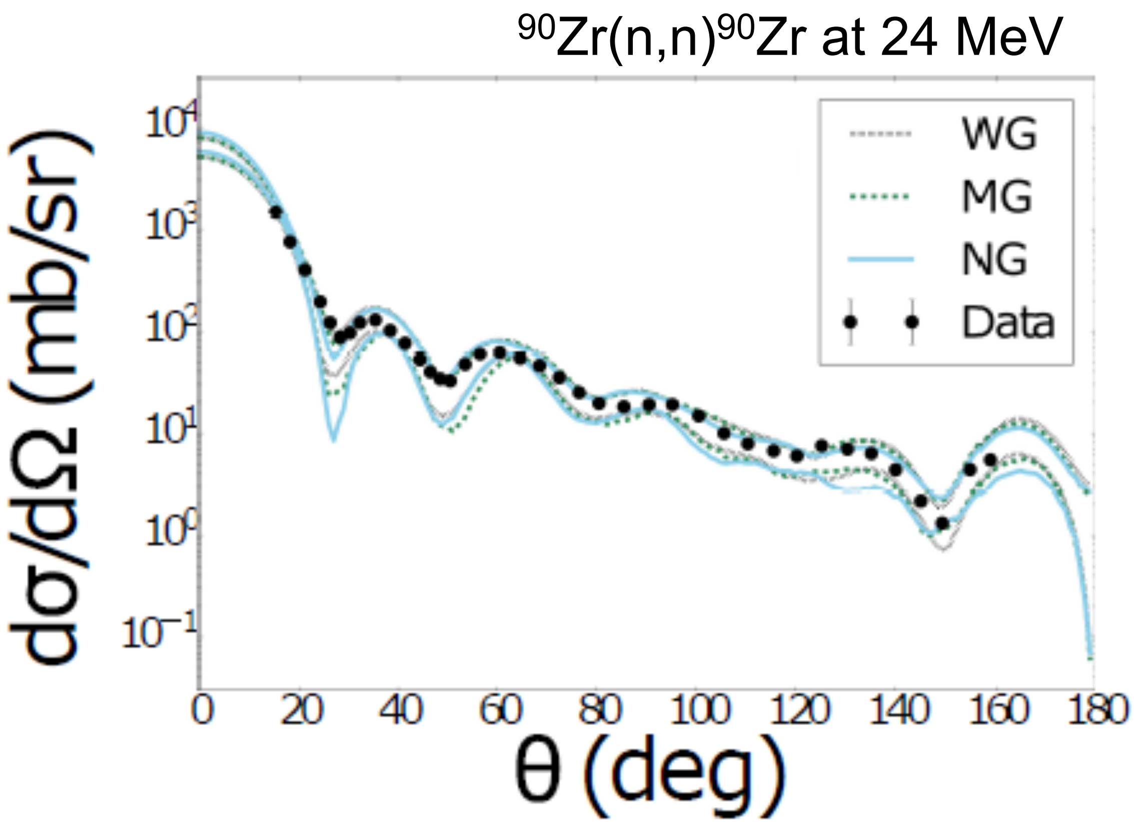
Wide (100% of original mean)

Medium (50% of original mean)

Narrow (10% of original mean)



Bayesian: prior dependence

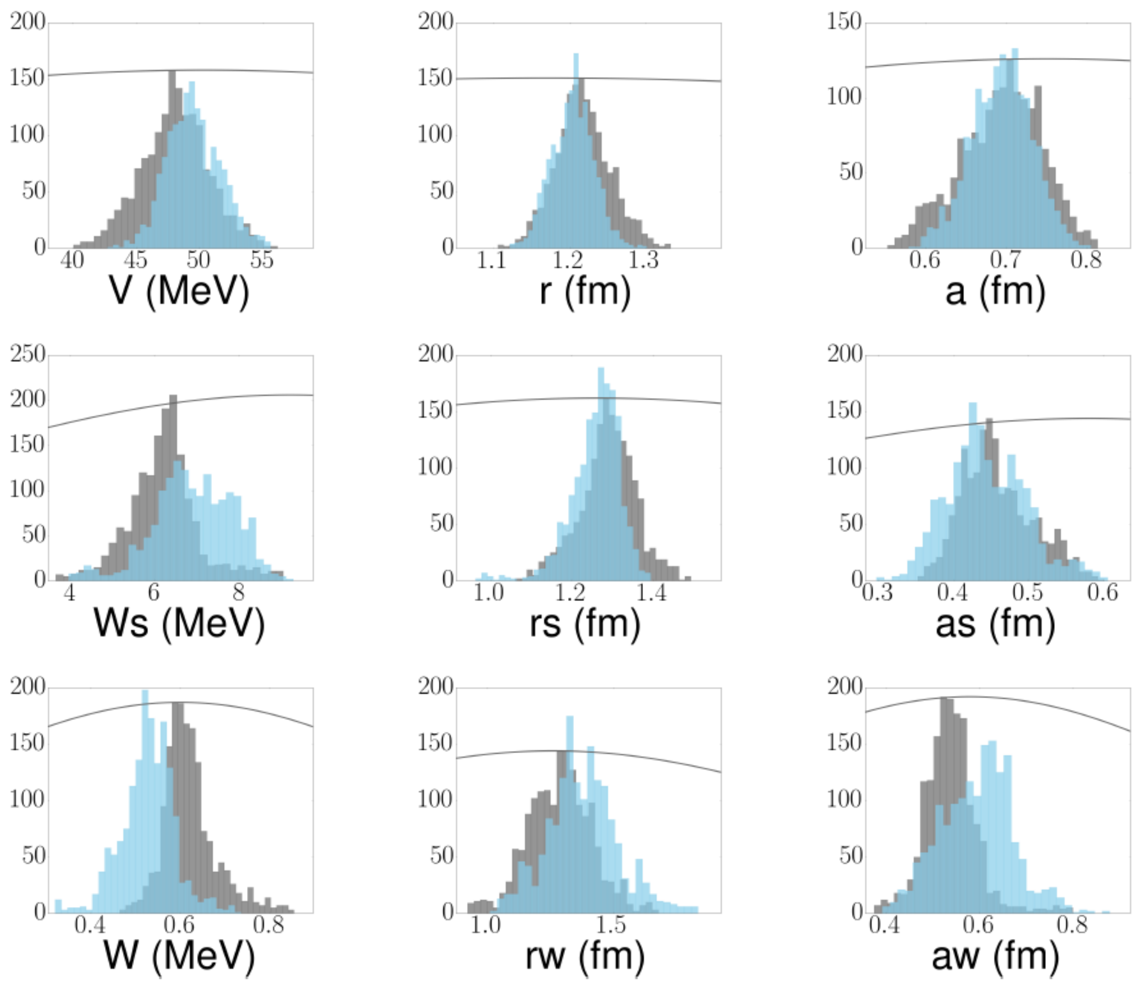


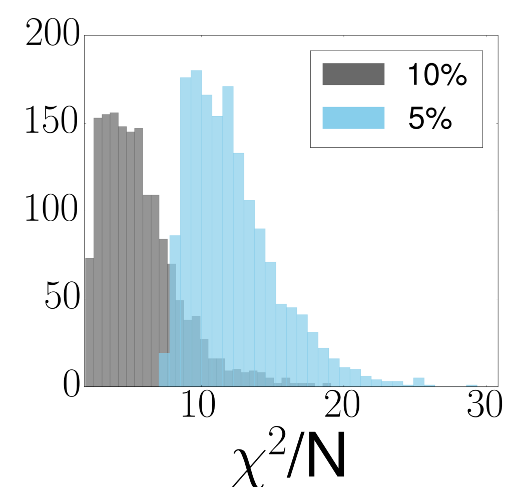
Types of Priors:
Wide (100% of original mean)
Medium (50% of original mean)
Narrow (10% of original mean)

Results independent of prior.
Data dominates over the prior.

Bayesian: optical potential

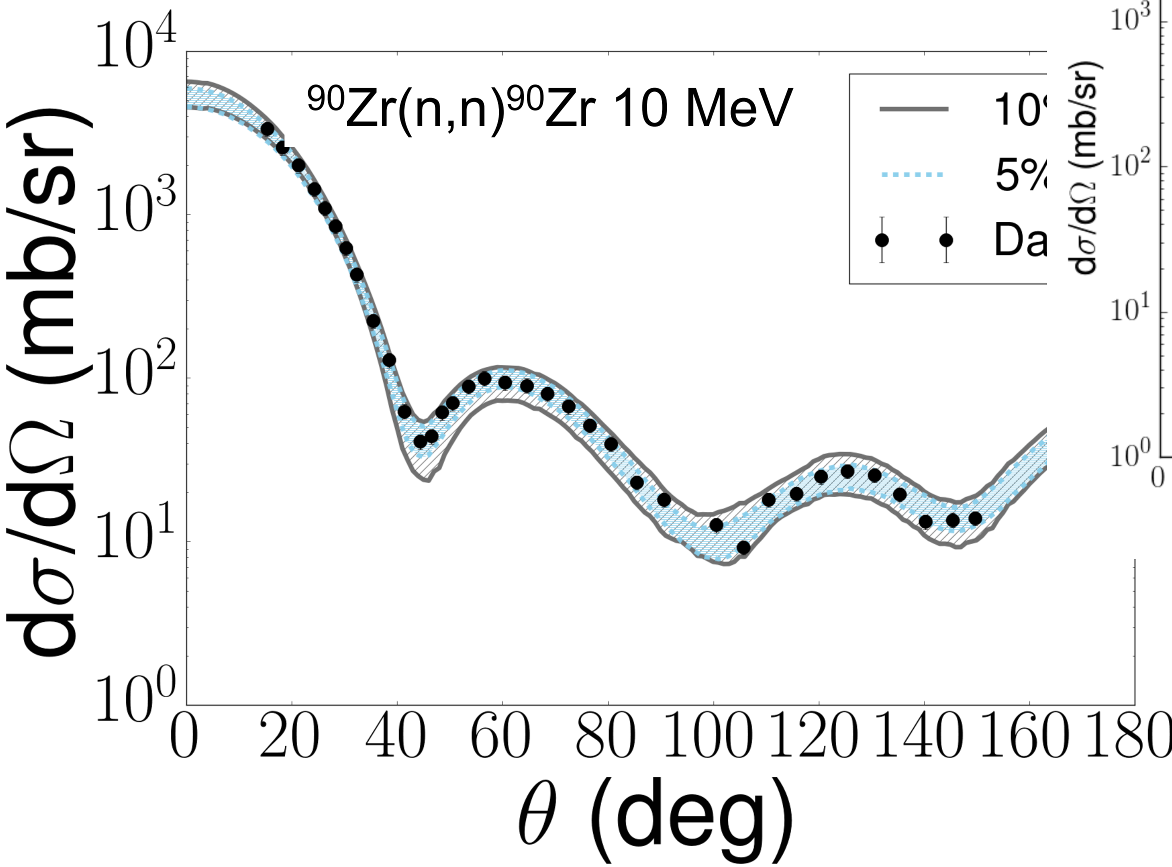
$^{90}Zr(n,n)^{90}Zr$ at 10 MeV

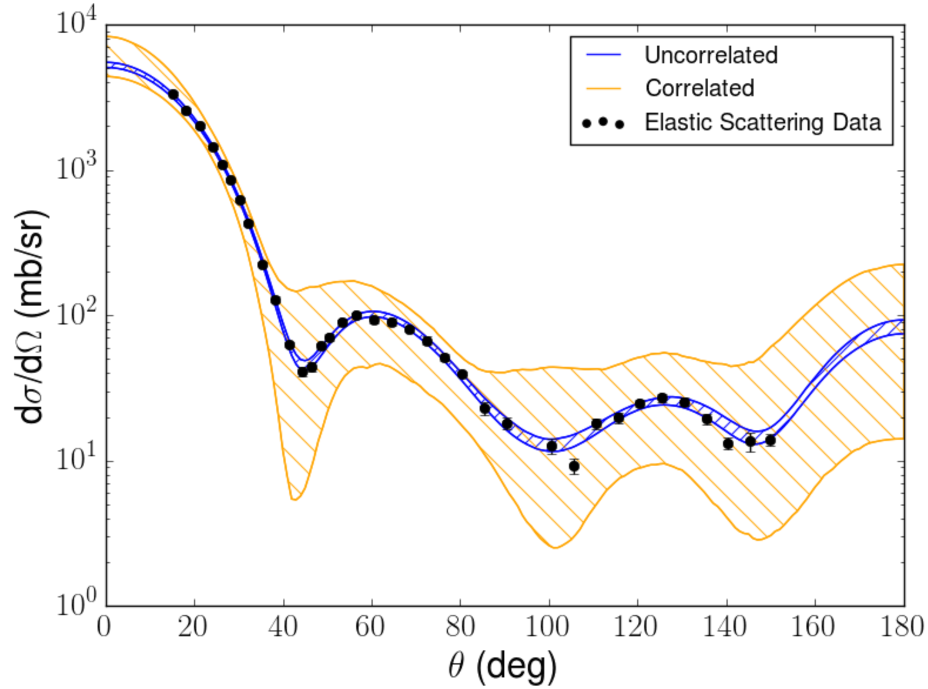




Uncorrelated Chi2	Correlated Chi2
V=50.6 MeV	V=51.9 MeV
r=1.18 fm	r=1.16 fm
a=0.63 fm	a=0.67 fm
Ws=3.3 MeV	Ws=4.1 MeV
Rs=1.06 fm	Rs=1.28 fm
as=0.80 fm	as=0.63 fm
W=0.6 fm	W=0.57 fm
rw=1.52 fm	rw=1.27 fm
aw=0.57 fm	aw=0.71 fm

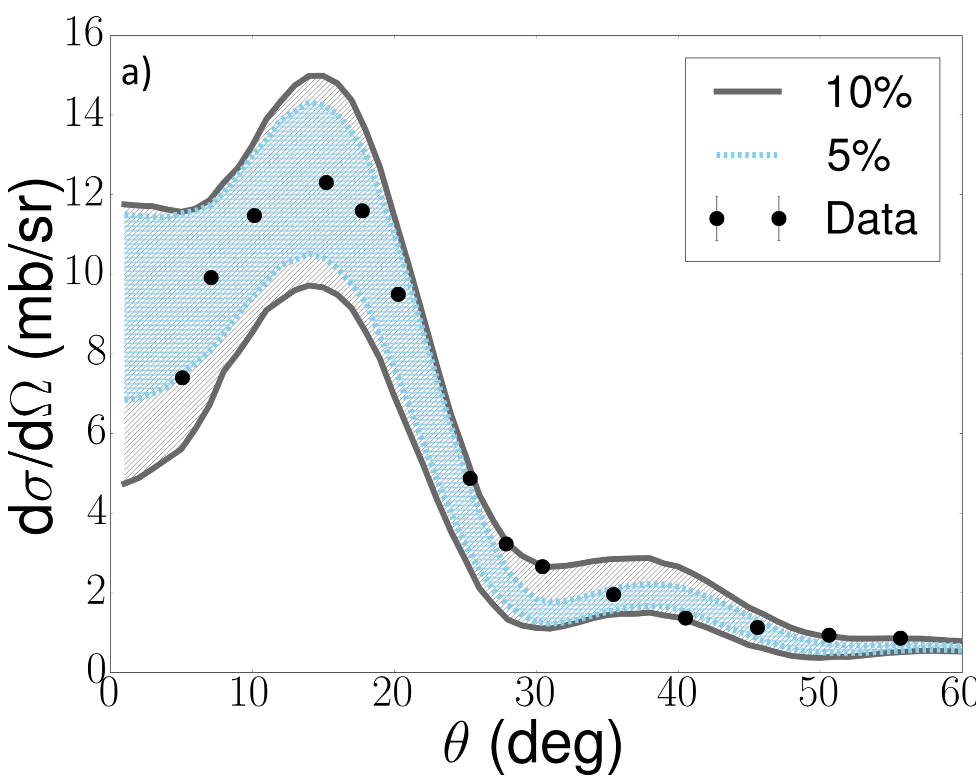
Bayesian: elastic scattering

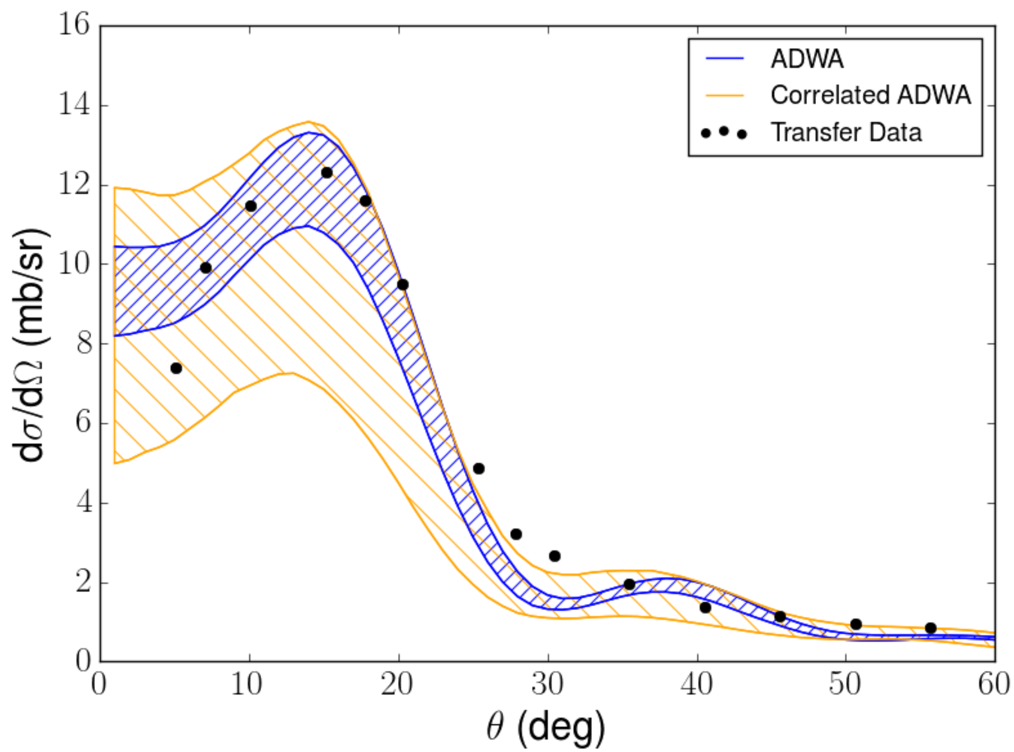




Bayesian: transfer predictions

$^{90}Zr(d,p)^{90}Zr$ at 24 MeV





Systematics with Bayesian

Reaction	Theory	θ (deg)	Peak* (mb/sr)	SF	ε_{95} (%)	ε_{68} (%)
^{48}Ca(d,p)	ADWA10	6	34.09	1.07	35.76	16.47
^{48}Ca(d,p)	ADWA5	6	33.38	1.09	24.24	11.53
^{48}Ca(d,p)	DWBA10	3	41.56	1.02	47.93	22.57
^{48}Ca(d,p)	DWBA5	4	40.73	1.02	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	0.74	47.62	21.95
^{90}Zr(d,p)	ADWA5	14	17.94	0.69	30.88	14.99
^{90}Zr(d,p)	DWBA10	16	17.09	0.72	58.86	29.02
^{90}Zr(d,p)	DWBA5	16	17.41	0.71	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

Conclusions

- Used elastic scattering to constrain OP and determine confidence bands on predicted transfer cross sections: compared the frequentist approach with Bayesian approach.
- Chi2 minimization: optical potentials obtained with correlated chi2 differ from uncorrelated chi2 and the correlated chi2 result in much wider confidence bands.
- Significant difference between DWBA and ADWA but uncertainty is still too large for data to discriminate between one or the other.

Conclusions

- Used elastic scattering to constrain OP and determine confidence bands on predicted transfer cross sections: compared the frequentist approach with Bayesian approach.

- Developed the Bayesian machinery to explore uncertainty quantification in reactions (including the Markov Chain Monte Carlo):
  - Results are independent of the prior – driven by data
  - Bayesian approach provides a picture closer to the correlated chi2 approach, but suggests correlations are more complex.

- Reducing errors bars from 10% to 5% produces a confidence band at most 30% narrower.

Outlook

- Parametrical uncertainties: we constrained all distorted waves in the problem. Still missing bound states – constrain mean field or ANC with other observables

- Diversify the data – currently just elastic angular distributions
  - Include reaction/total cross sections, polarization data, other channels
  - Principal component analysis to determine information content of data

- Model comparison and model mixing

Outlook

- Importance of explicit inclusion of nonlocality calls for new global nonlocal potential

- Initial work on n+A and p+A demonstrates that, when including a Gaussian nonlocality, elastic scattering data still calls for an energy dependence of the interaction.

- Bayesian techniques provide an avenue for a comprehensive study

Thank you for your attention!

In collaboration with:
Amy Lovell, Garrett King (MSU)
Stephan Wild and Jason Sarich (ANL)

Supported by: NNSA-DOE, NSF