Status and plans for ^{1}H and ^{16}O evaluations by R-matrix analyses of the *NN* and ^{17}O systems

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Outline

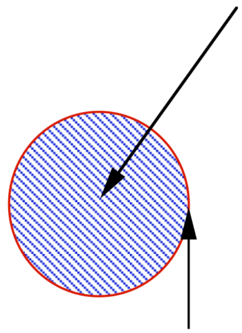
- Introduction to R-matrix theory, EDA code
- Status of N-N (n-p) scattering analysis up to 30 MeV
- Summary of N-N data available at higher energies
- Current status of n+^{16}O (^{17}O system) analysis
- Example of unitary constraints on cross sections
- More recent work on ^{17}O
- Plans for future work on NN, ^{17}O systems
- Some thoughts on small parameter uncertainties

Schematic of R-matrix Theory

INTERIOR (Many-Body) REGION
(Microscopic Calculations)

$\underbrace{H + \mathcal{L}_B}$

compact, hermitian operator with real, discrete spectrum; eigenfunctions in Hilbert space



$$|\psi^+) = (H + \mathcal{L}_B - E)^{-1} \mathcal{L}_B |\psi^+)$$

SURFACE

$$\mathcal{L}_B = \sum_c |c)(c| \left(\frac{\partial}{\partial r_c} r_c - B_c \right),$$

$$(\mathbf{r}_c | c) = \frac{\hbar}{\sqrt{2\mu_c a_c}} \frac{\delta(r_c - a_c)}{r_c} [(\phi_{s_1}^{\mu_1} \otimes \phi_{s_2}^{\mu_2})_s^{\mu} \otimes Y_l^m(\hat{\mathbf{r}}_c)]_J^M$$

$$R_{c'c} = (c' | (H + \mathcal{L}_B - E)^{-1} | c) = \sum_\lambda \frac{(c' | \lambda)(\lambda | c)}{E_\lambda - E}$$

ASYMPTOTIC REGION
(S-matrix, phase shifts, etc.)

$$\left(r_{c'} \middle| \psi_c^+ \right\rangle = -I_{c'}(r_{c'}) \delta_{c'c} + O_{c'}(r_{c'}) S_{c'c}$$

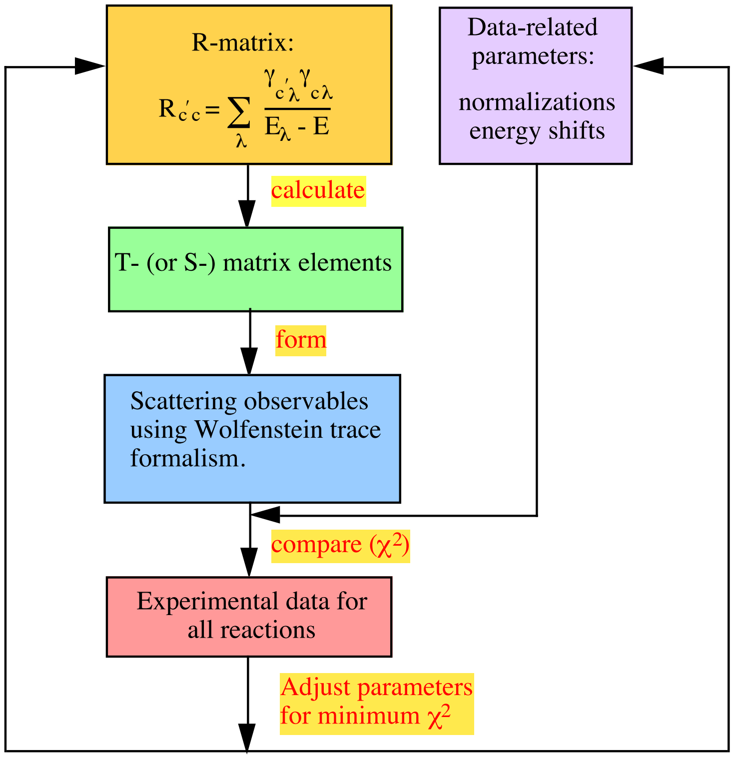
or equivalently,

$$\left(r_{c'} \middle| \psi_c^+ \right\rangle = F_{c'}(r_{c'}) \delta_{c'c} + O_{c'}(r_{c'}) T_{c'c}$$

Measurements

Some properties of EDA:

Energy Dependent Analysis Code



- Accommodates general (spins, masses, charges) two-body channels
- Uses relativistic kinematics and R-matrix formulation
- Calculates general scattering observables for 2 ➔2 processes
- Has rather general data-handling capabilities (but not as general as, e.g., SAMMY)
- Uses modified variable-metric algorithm that gives parameter covariances at a solution

Charge-Independent Analysis of *N*-*N* Scattering up to 30 MeV

Channel	a_c (fm)	l_{max}
p+p	3.26	3
n+p	3.26	3
γ+d	40	1

Reaction	# Pts.	χ^2	Observable Types
p(p,p)p	692	815	$\sigma(\theta)$, $A_y(p)$, $C_{x,x}$, $C_{y,y}$, $K_x^{x'}$, $K_y^{y'}$, $K_z^{x'}$
p(n,n)p	4378	3232	σ_T, $\sigma(\theta)$, $A_y(n)$, $C_{y,y}$, $K_y^{y'}$
p(n,γ)d	80	133	σ_{int}, $\sigma(\theta)$, $A_y(n)$
d(γ,n)p	59	35	σ_{int}, $\sigma(\theta)$, $\Sigma(\gamma)$, $P_y(n)$
Norms.	129	72	
Total	5338	4287	19

free parameters = 44+129 ⇒ χ^2/degree of freedom = 0.830

n-p Scattering Lengths

From the analysis,

a_0 = -23.719(5) fm, a_1 = 5.414(1) fm,

giving

$a_c = (3a_1 + a_0)/4 = -1.8693$ fm,

$\sigma_{pol} = (a_1^2 - a_0^2)/4 = -1.3332$ b,

$\sigma_{sc} = \pi(3a_1^2 + a_0^2) = 20.437$ b.

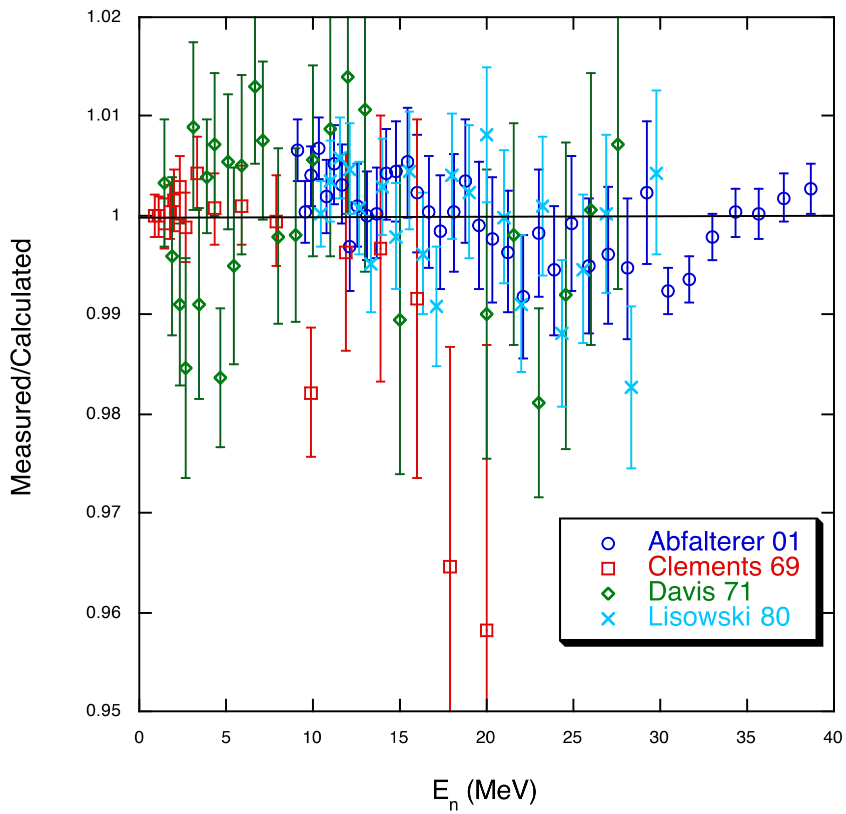
The first two agree exactly with experimental values, while the last one agrees with the measurement of Houk, (20.436 ± 0.023) b, but not with that of Dilg, (20.491 ± 0.014) b.

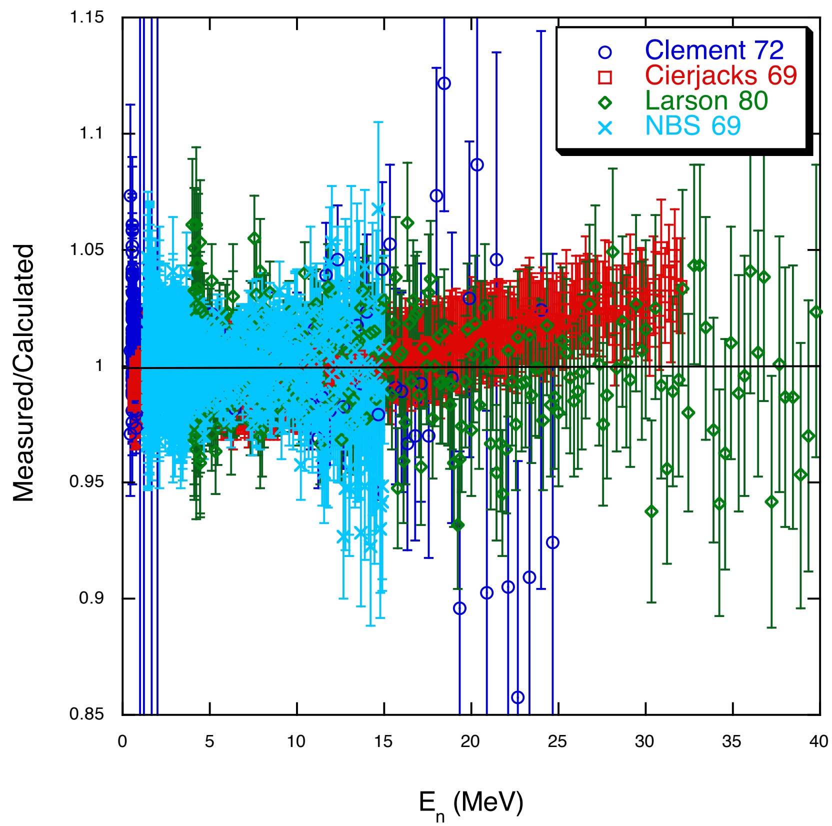
The spin-dependent scattering lengths from AV_{18} are

a_0 = -23.732 fm, a_1 = 5.419 fm,

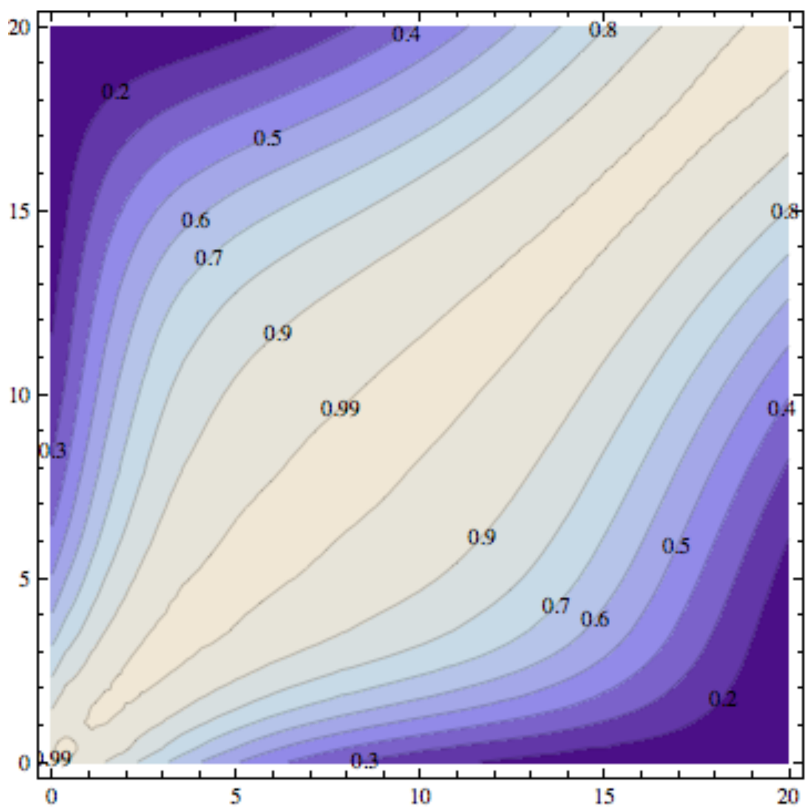
in good agreement with those from the analysis.

n-p Total Cross Sections

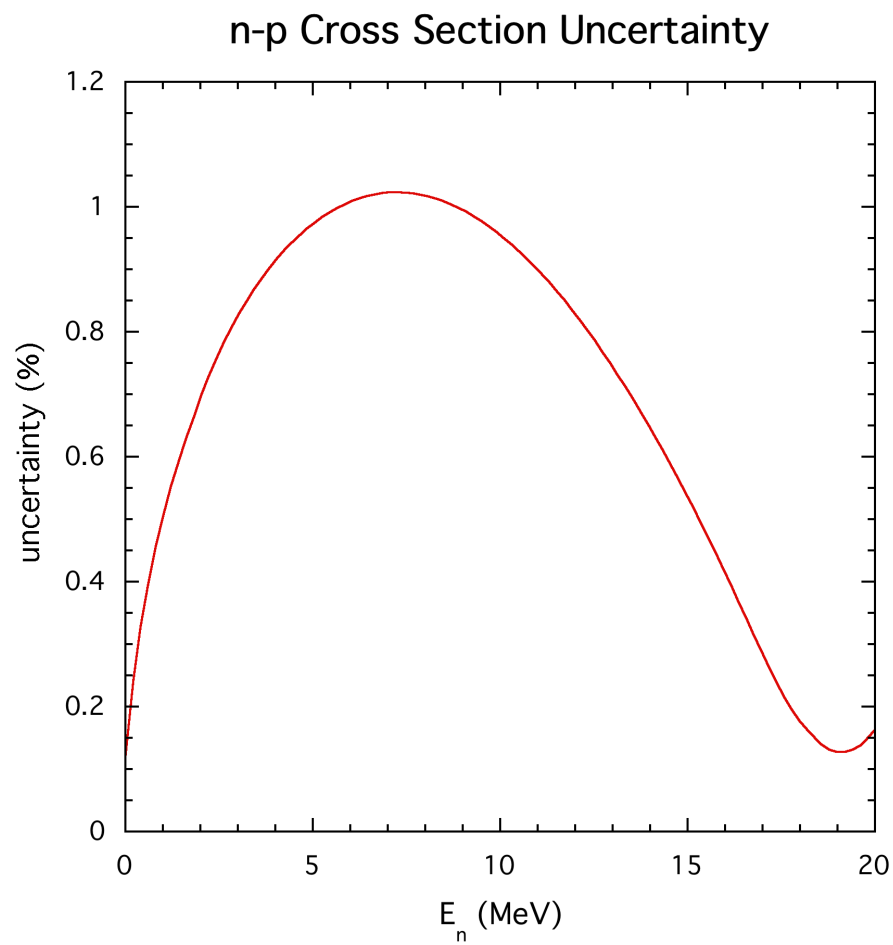




Covariances for n-p Scattering Cross Sections



$\rho_{nn}(E,E')$



N-N Data Available at Higher Energies

	0 < E < 30 MeV														
	$\sigma(\theta)$	P_{n000}	D_{n0n0}	K_{0nn0}	A_{00nn}	A_{00ss}	A_{00kk}	A_{00sk}	$C_{\ell m00}$	$D_{s'0s0}$	$D_{k'0s0}$	$K_{0s''s0}$	$D_{s'0k0}$	$D_{k'0k0}$	$K_{0s''k0}$
	$\sigma(\theta)$	P	D	D_T	A_{yy}	A_{xx}	A_{zz}	A_{zx}	C_{KP}	R	R_P	R_T	A	A_P	A_T
pp	363	70	8	0	7	4	0	0	0	8	0	0	5	0	0
np	243	231	0	3	31	0	0	0	0	0	0	0	0	0	0

	30 MeV < E < 150 MeV														
	$\sigma(\theta)$	P_{n000}	D_{n0n0}	K_{0nn0}	A_{00nn}	A_{00ss}	A_{00kk}	A_{00sk}	$C_{\ell m00}$	$D_{s'0s0}$	$D_{k'0s0}$	$K_{0s''s0}$	$D_{s'0k0}$	$D_{k'0k0}$	$K_{0s''k0}$
	$\sigma(\theta)$	P	D	D_T	A_{yy}	A_{xx}	A_{zz}	A_{zx}	C_{KP}	R	R_P	R_T	A	A_P	A_T
pp	331	257	24	0	8	3	0	0	1	24	14	0	21	0	0
np	629	313	0	6	28	0	20	0	0	5	0	0	5	0	3

	150 MeV < E < 250 MeV														
	$\sigma(\theta)$	P_{n000}	D_{n0n0}	K_{0nn0}	A_{00nn}	A_{00ss}	A_{00kk}	A_{00sk}	$C_{\ell m00}$	$D_{s'0s0}$	$D_{k'0s0}$	$K_{0s''s0}$	$D_{s'0k0}$	$D_{k'0k0}$	$K_{0s''k0}$
	$\sigma(\theta)$	P	D	D_T	A_{yy}	A_{xx}	A_{zz}	A_{zx}	C_{KP}	R	R_P	R_T	A	A_P	A_T
pp	60	203	28	8	96	96	39	96	0	23	11	0	20	5	0
np	456	164	5	13	39	0	2	0	0	0	0	7	0	0	7

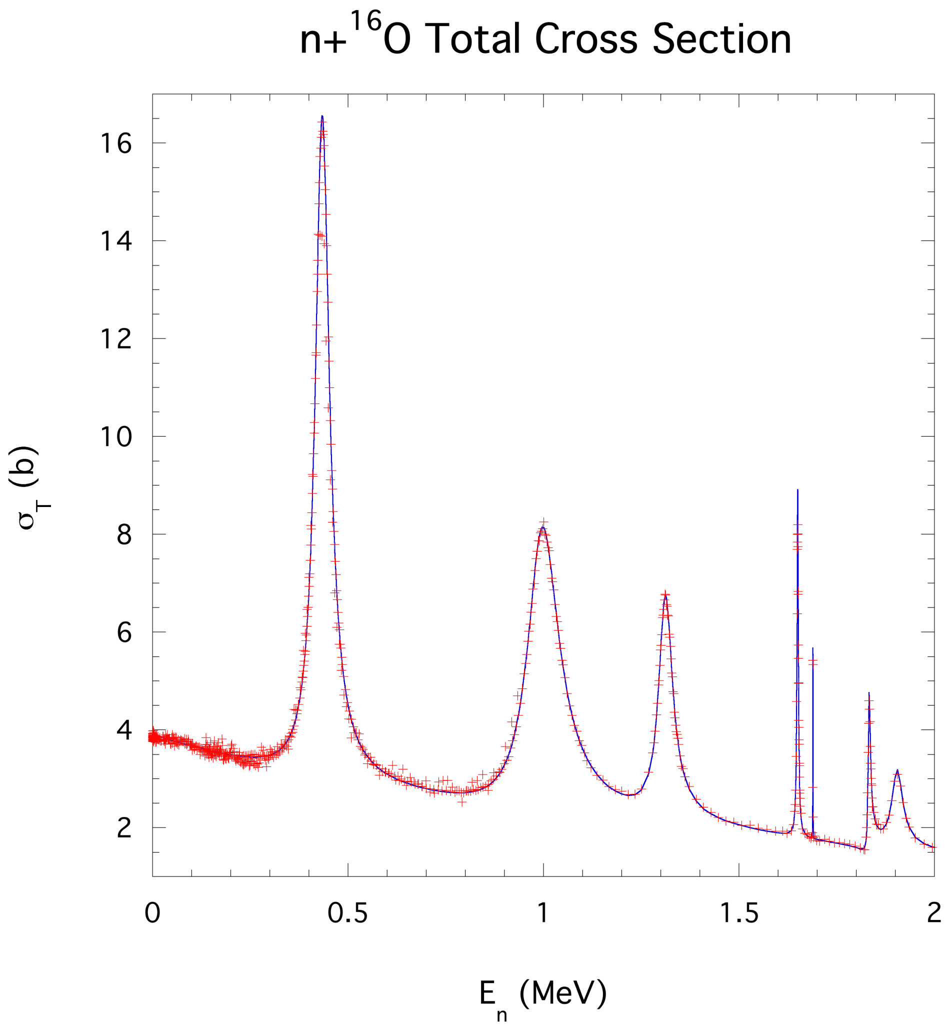
Measured	Unp. beam/Unp. target	Pol. beam/Unp. target	Unp. beam/Pol. target	Pol. beam/Pol. target
Differential cross section	I_{0000}	A_{0000}	A_{000k}	A_{00ik}
Scatt. pol.	P_{p000}	D_{p0i0}	K_{p00k}	M_{p0ik}
Recoil pol.	P_{0q00}	K_{0qi0}	D_{0q0k}	N_{0qik}
Pol. correlations	C_{pq00}	C_{pqi0}	C_{pq0k}	C_{pqik}

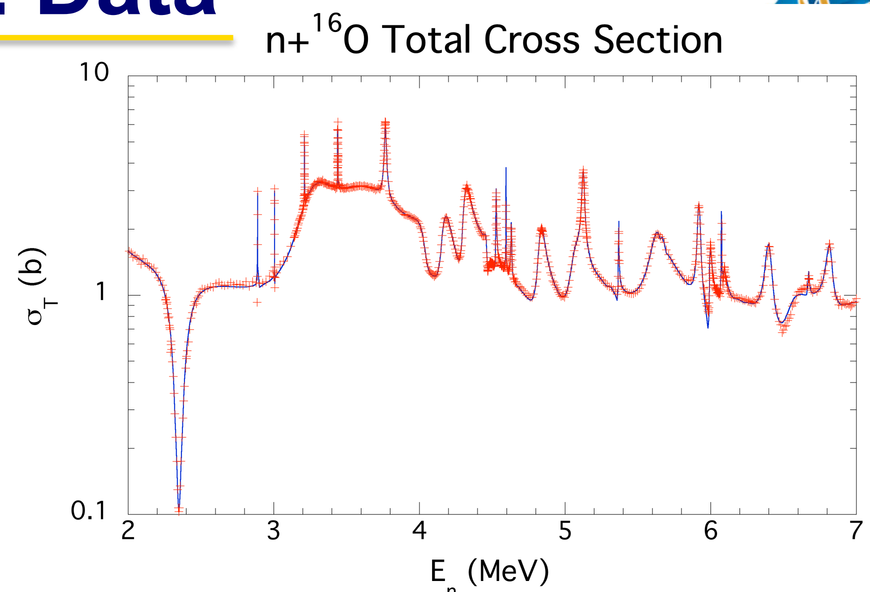
R-Matrix Analysis of Reactions in the ^{17}O System

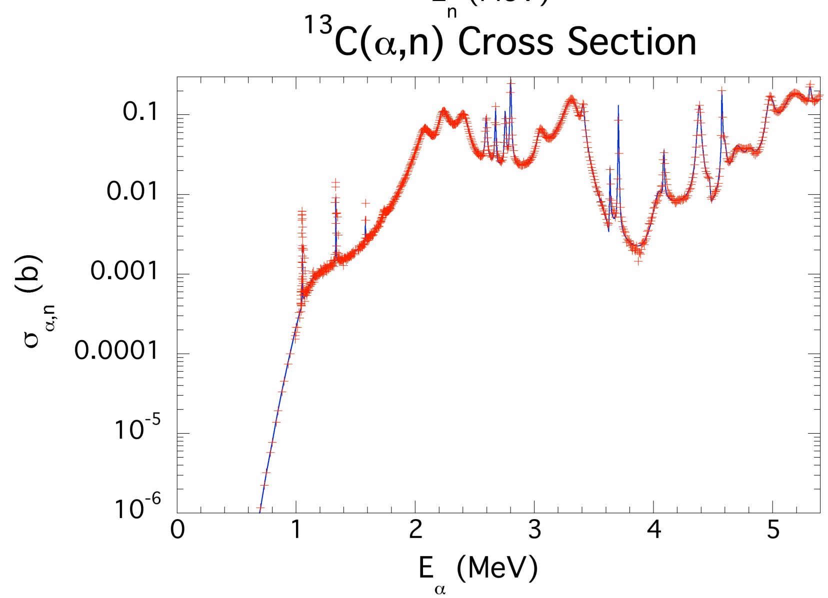
channel	a_c (fm)	l_{max}
n+^{16}O	4.3	4
α+^{13}C	5.4	5

Reaction	Energies (MeV)	# data points	Data types
$^{16}O(n,n)^{16}O$	$E_n = 0 – 7$	2718	σ_T, $\sigma(\theta)$, $P_n(\theta)$
$^{16}O(n,\alpha)^{13}C$	$E_n = 2.35 – 5$	850	σ_{int}, $\sigma(\theta)$, $A_n(\theta)$
$^{13}C(\alpha,n)^{16}O$	$E_\alpha = 0 – 5.4$	874	σ_{int}
$^{13}C(\alpha,\alpha)^{13}C$	$E_\alpha = 2 – 5.7$	1296	$\sigma(\theta)$
total		5738	8

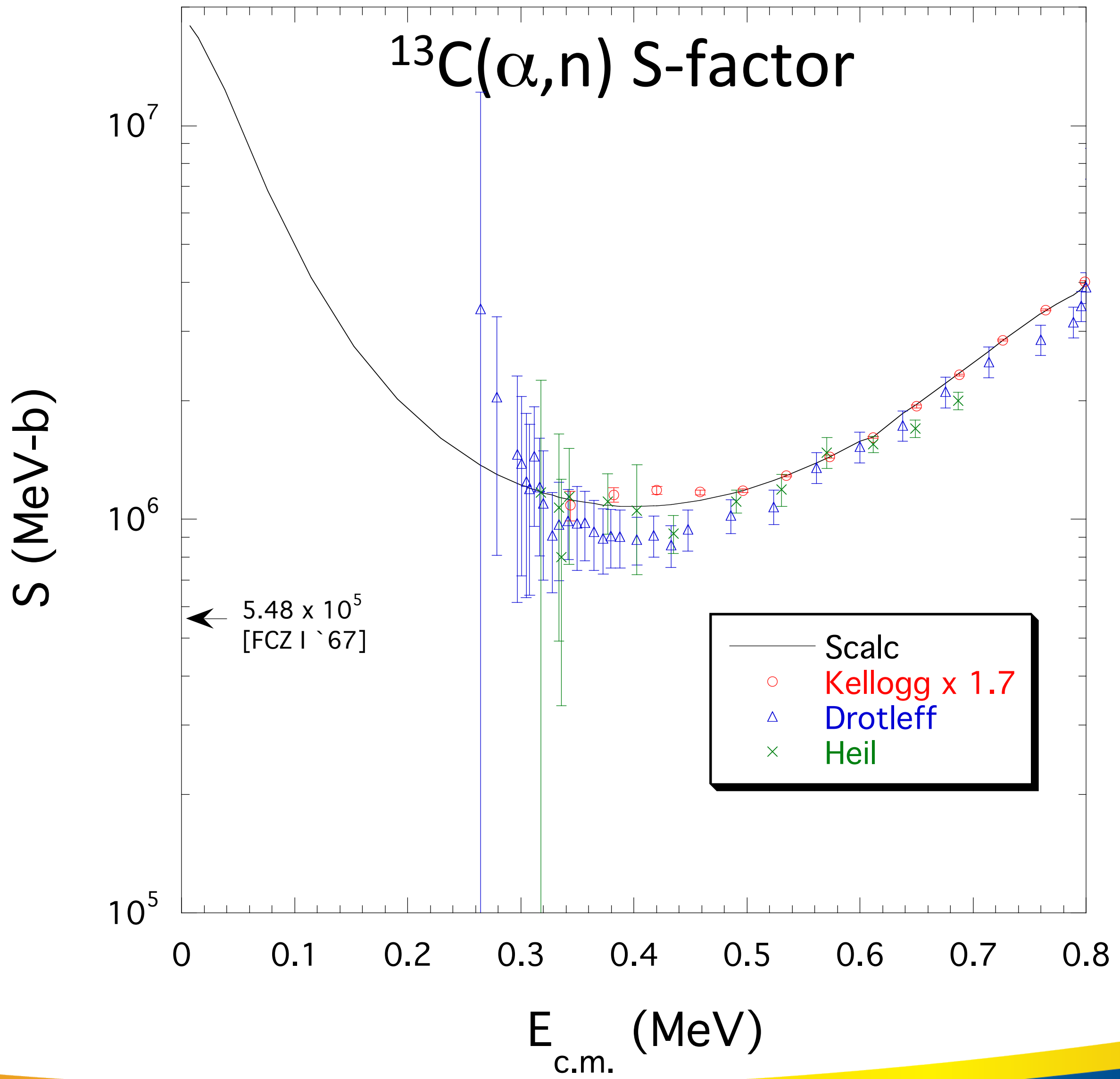
Comparisons with Exptl. Data



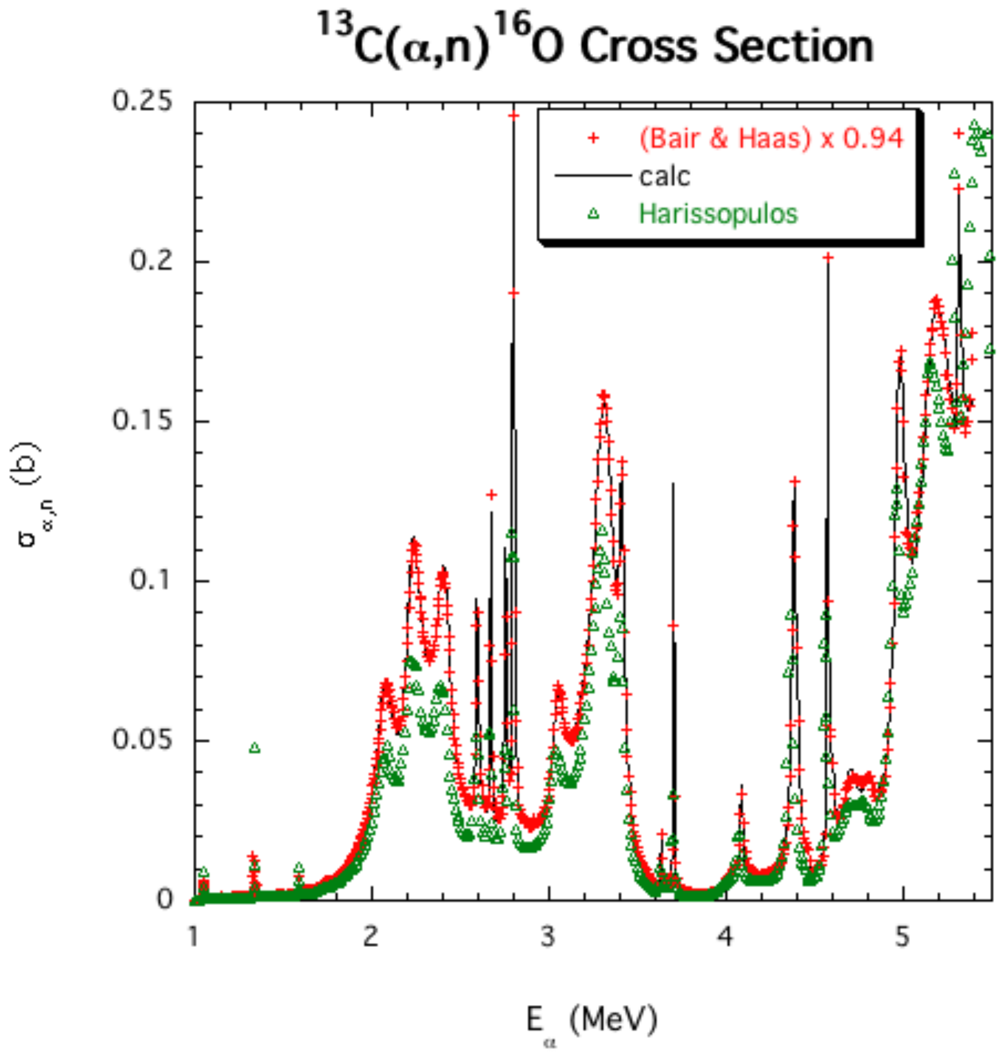




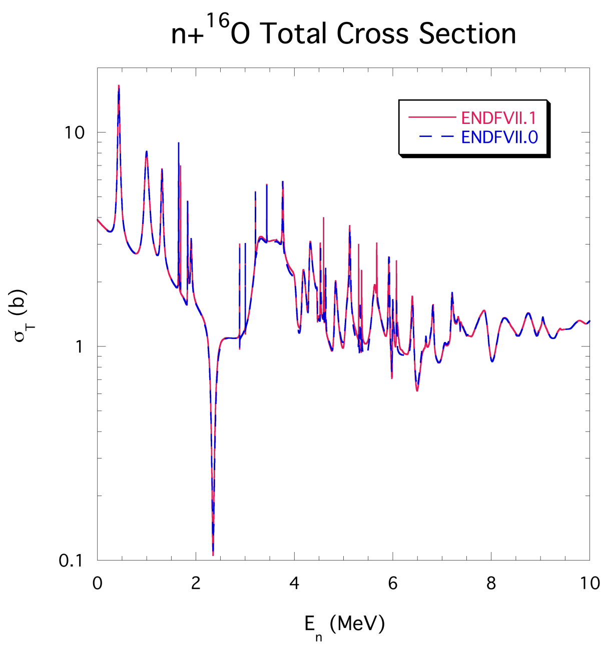
Comparisons with Exptl. Data, Cont.

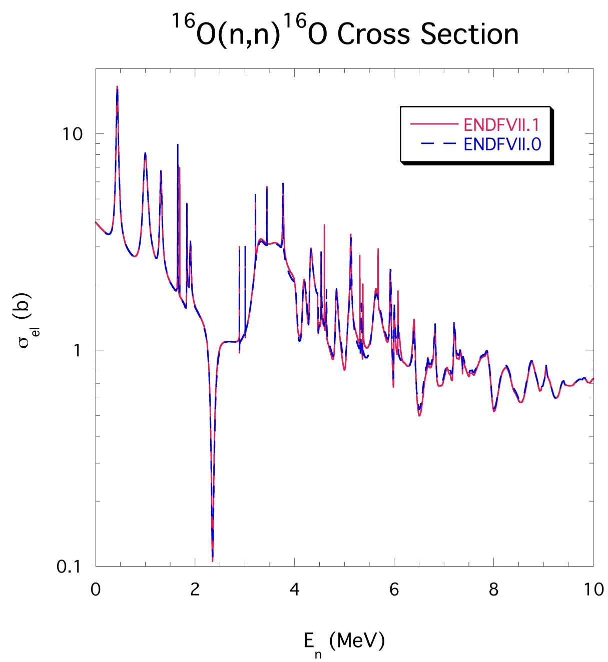


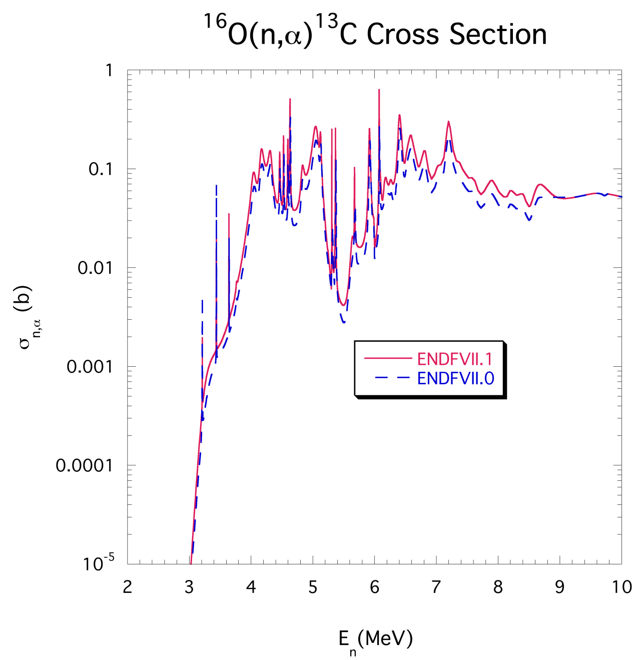
Comparisons with Exptl. Data, Cont.



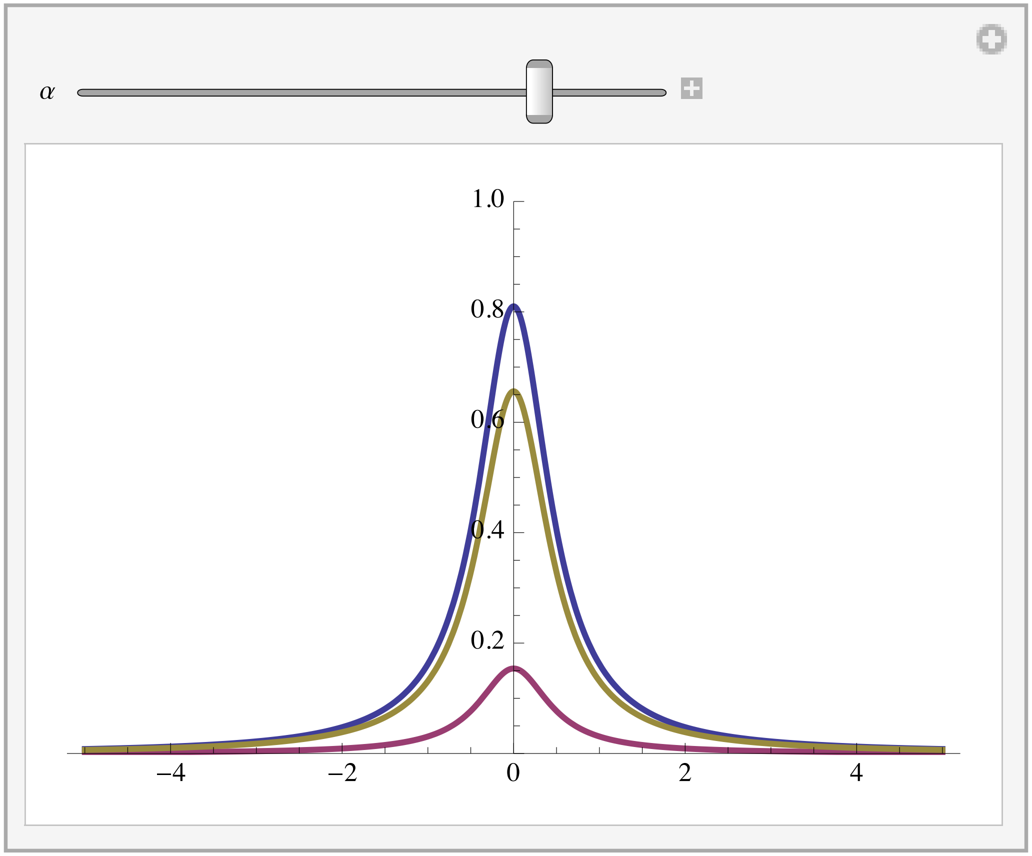
Comparisons with ENDF/B VII.1







Cross Sections Calculated from a Unitary Theory



Recent EDA Work on ^{17}O System

- Okhubo σ_T data, corrected for ^{1}H content (by Plompen, Kopecky), replaced original

  → $\sigma_T(0) \approx 3.8$ b
- Calculated σ_T allowed to over-shoot data in many peaks using csqmax=10

  → calculated σ_R reduced ~ 15%

  This suggests that resolution corrections are important to consider in the connection of unitarity to experimental normalizations

Plans for Future LANL Work on N-N, ^{17}O Systems

- Add new data to N-N analysis (including n-p capture and d-photo-disintegration data), increasing the energy range by ~ 50 MeV steps, until we have reached at least 200 MeV. Target date for completion is October 2014.

- Continue ^{17}O analysis with all charged-particle data presently included, and neutron data as suggested/corrected by the CIELO working sub-group. Examine carefully the effects of unitarity and experimental resolution on the normalizations of the experimental data sets included in the analysis. Target date for completing this analysis is March 2014.

Uncertainties from Chi-Squared Minimization

$$\chi^2_{\mathrm{EDA}} = \sum_i \left[\frac{nX_i(\mathbf{p}) - R_i}{\Delta R_i}\right]^2 + \left[\frac{nS-1}{\Delta S / S}\right]^2 \quad \begin{cases} R_i,\ \Delta R_i = \text{relative measurement, uncertainty} \\ S,\ \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{cases}$$

Near a minimum of the chi-squared function at $\mathbf{p} = \mathbf{p}_0$,

$$\begin{aligned} \chi^2(\mathbf{p}) &= \chi_0^2 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0) \\ &= \chi_0^2 + \Delta\chi^2. \end{aligned} \quad \begin{cases} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

$$\Delta\chi^2 = \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0) = \tfrac{1}{2}\Delta\mathbf{p}^{\mathrm{T}}\mathbf{G}_0\Delta\mathbf{p}$$

is a chi-square distribution function with *k* degrees of freedom.

Parameter Covariance Matrix

A multivariate normal distribution function of the form

$$f_k(\Delta\mathbf{p}) = \sqrt{\frac{|\mathbf{G}_0|}{(4\pi)^k}} \exp(-\tfrac{1}{4}\Delta\mathbf{p}^{\mathrm{T}}\mathbf{G}_0\Delta\mathbf{p})$$

would have the parameter covariance matrix

$$\mathbf{C}_{\mathbf{p}} = \left\langle \Delta\mathbf{p}\Delta\mathbf{p}^{\mathrm{T}} \right\rangle = 2\mathbf{G}_0^{-1} = 2\mathbf{H},$$

and therefore parameter uncertainties $\sigma_{p_i} = \sqrt{2H_{ii}}$.

These uncertainties can become much less than 1% for problems with large experimental data sets, and lead to unrealistically small propagated errors in the calculated cross sections.

Parameter Confidence Intervals

It was proposed by Y. Avni [*Ap. J.* **210**, 642 (1976)] to define confidence intervals for the parameters of a fit by the condition

$$\Delta\chi^2 = \tfrac{1}{2}\Delta\mathbf{p}^{\mathrm{T}}\mathbf{G}_0\Delta\mathbf{p} \le \Delta\chi^2_{\mathrm{max}},$$

where $\Delta\chi^2_{\mathrm{max}}$ is chosen to give a particular confidence level (CL)

$$P(\Delta\chi^2 \,|k) = \left[2^{\frac{k}{2}}\Gamma(\tfrac{k}{2})\right]^{-1} \int_0^{\Delta\chi^2_{\mathrm{max}}} t^{\frac{k}{2}-1} e^{-\frac{t}{2}} dt = \mathrm{CL}\ (\text{e.g.} \sim 0.68 \text{ for } 1\text{-}\sigma),\ 0.95 \text{ for } 2\text{-}\sigma, \text{etc.}$$

for a chi-squared distribution with *k* degrees of freedom. Many statistical analysis (not necessarily physical science) applications use this method to determine parameter uncertainties (usually with CL = 95%, or 2-σ). For CL = 68% (1-σ), $\Delta\chi^2_{\mathrm{max}} \approx k = \langle \Delta\chi^2 \rangle$, and the fitting program `NonlinearModelFit` in *Mathematica* gives parameter confidence levels nearly the same as the standard errors, $\sigma_{\mathbf{p}}$, when *k* is small. How does this look for larger *k*? Should we be using confidence intervals instead of standard deviations? We will continue to study this question.