LA-UR-16-29052

A MODERN THEORETICAL APPROACH TO THE R-MATRIX AND THE COMING EDA6 LOS ALAMOS IMPLEMENTATION

Los Alamos NATIONAL LABORATORY EST. 1943

M. Paris & G. Hale (T-2, Los Alamos National Lab)

Outline

- Overview
  - History at LANL
  - Updated analyses
- Modern Green-function R-matrix formalism
  - Bloch formalism: single-channel; multichannel
  - Multichannel unitarity
  - Relativistic parametrization
- EDA6
  - Code features & desiderata
- Resonance parameters
  - Brune alternative parametrization
  - vs. S-/T-matrix poles

<u>An immodest proposal:</u>
Consider the model independent S-/T-matrix poles for verification of analyses

Overview of multichannel reaction analysis

- History of **E**nergy **D**ependent **A**nalysis
  - Developers: D. Dodder, K. Witte, G. Hale, A. Sierk, MP
  - originally motivated by hadronic analyses e.g. $\pi N \rightarrow \pi N$
    - Origin of relativistic parametrization
  - EDA5 F77; EDA6 F90/95 (targeted for '17)
- Overview
  - EDA5/6 implement Wigner/Eisenbud/Bloch phenomenological R matrix
  - Handles large number of two-body partitions & channels, including EM
  - Data: elastic, inelastic, reaction; diff'l, integrated, total, polarization
- Existing analyses to date…

EDA Existing Analyses

A	System	Channels	Energy Range (MeV)
2	N-N	p+p; n+p, γ+d	0-30 0-40
3	N-d	p+d; n+d	0-4
4	^{4}H ^{4}Li	n+t p+^{3}He	0-20
	^{4}He	p+t n+^{3}He d+d	0-11 0-10 0-10
5	^{5}He	n+α d+t ^{5}He+γ	0-28 0-10
	^{5}Li	p+α d+^{3}He	0-24 0-1.4

EDA Existing Analyses, Cont.

A	System (Channels)
6	^{6}He (^{5}He+n, t+t); ^{6}Li (d+^{4}He, t+^{3}He); ^{6}Be (^{5}Li+p, ^{3}He+^{3}He)
7	^{7}Li (t+^{4}He, n+^{6}Li); ^{7}Be (γ+^{7}Be, ^{3}He+^{4}He, p+^{6}Li)
8	^{8}Be (^{4}He+^{4}He, p+^{7}Li, n+^{7}Be, p+^{7}Li*, n+^{7}Be*, d+^{6}Li)
9	^{9}Be (^{8}Be+n, d+^{7}Li, t+^{6}Li); ^{9}B (γ+^{9}B, ^{8}Be+p, d+^{7}Be, ^{3}He+^{6}Li)
10	^{10}Be (n+^{9}Be, ^{6}He+α, ^{8}Be+nn, t+^{7}Li); ^{10}B (α+^{6}Li, p+^{9}Be, ^{3}He+^{7}Li)
11	^{11}B (α+^{7}Li, α+^{7}Li*, ^{8}Be+t, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
12	^{12}C (^{8}Be+α, p+^{11}B)
13	^{13}C (n+^{12}C, n+^{12}C*)
14	^{14}C (n+^{13}C)
15	^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
16	^{16}O (γ+^{16}O, α+^{12}C)
17	^{17}O (n+^{16}O, α+^{13}C)
18	^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

Recent updates (listed by target nucleus)

^{1}H: (n,n), (n,γ) < 200 MeV

^{6}Li: (n,n), (t,t), (t,n) E_t<14 MeV; (n,n),(n,t),(n,d) E_n<4 MeV

^{7}Be: elastic, (n,γ), (n,tot), (n,α) <20 MeV

^{9}Be: angular distributions

^{10}B: < 5 MeV

^{12}C: elastic, (n,tot), (n,n') < 6.5 MeV

^{13}C: (n,tot), (n,γ) < 20 MeV

^{16}O: elastic, (n,α), (n,tot), (n,γ) < 9 MeV

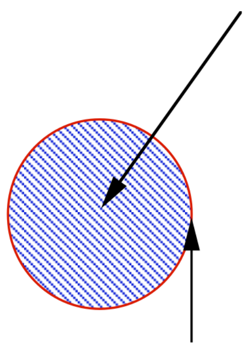
The canonical EDA "modern" R-matrix slide

$\mathscr{I}$

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

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

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

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

$\mathscr{E}$

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

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

or equivalently,

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

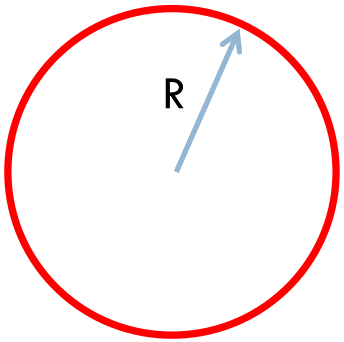
Measurements

Toy model example: single channel, s-wave, neut.

First solve a problem with a simple BC:

$$(H - E_\lambda)\psi_\lambda(r) = 0$$

$$\frac{d}{dr} r\psi_\lambda(r)\Big|_{r=a} = 0$$



Q: What is the spectrum?

$$\int_0^R r^2 dr [\psi_1^*(H\psi_2) - (H\psi_1)^*\psi_2] = -\frac{\hbar^2}{2M}\left[r\psi_1^* \frac{d(r\psi_2)}{dr} - \frac{d(r\psi_1^*)}{dr} r\psi_2\right]_R$$

A: The above defines a Sturm-Liouville eigenvalue problem implying E_λ are *discrete* – and so ***not a scattering problem***

Two essential points

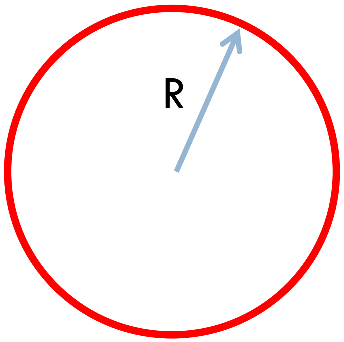
1. Scattering states in general don't satisfy the BC above
2. This implies that the E_λ are not simply related to resonance E

Toy model example: single channel, s-wave, neut.

<u>Now solve it with a more general BC:</u>

$$(H - E_\lambda)\psi_\lambda(r) = 0$$

$$\frac{d}{dr} r\psi_\lambda(r)\Big|_{r=a} = B$$



Caveat Emptor: No longer a S-L problem

$$\int_0^R r^2 dr[\psi_1^*(H\psi_2) - (H\psi_1)^*\psi_2] = -\frac{\hbar^2}{2M}\left[r\psi_1^*\frac{d(r\psi_2)}{dr} - \frac{d(r\psi_1^*)}{dr} r\psi_2\right]_R$$

The RHS doesn't vanish: eigenfunctions not orthogonal

Bloch "fixed" this issue.

Claude Bloch’s 1957 paper modernized R-matrix

UNE FORMULATION UNIFIÉE DE LA THÉORIE DES RÉACTIONS NUCLÉAIRES

CLAUDE BLOCH

Centre d’Études Nucléaires de Saclay, Gif-sur-Yvette (S. & O.)

Reçu le 13 avril 1957

A unified formulation of the theory of nuclear reactions

Claude Bloch[1]

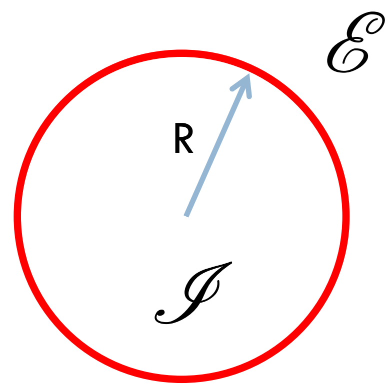
Centre d’Études Nucléaires de Saclay, Gif-sur-Yvette (S. & O.)

$$\int_0^R r^2 dr[\psi_1^*(H\psi_2) - (H\psi_1)^*\psi_2] = -\frac{\hbar^2}{2M}\left[r\psi_1^*\frac{d(r\psi_2)}{dr} - \frac{d(r\psi_1^*)}{dr}r\psi_2\right]_R$$

NB: The quantity B must be a real constant, indep. of energy in order to obtain an orthonormal basis

$$\mathscr{H} = H + \frac{\hbar^2}{2MR}\delta(r-R)\left[\frac{d}{dr}r - \frac{B}{r}\right]$$

$$\int_0^R r^2 dr\,[\psi_1^*(\mathscr{H}\psi_2) - (\mathscr{H}\psi_1)^*\psi_2] = 0.$$



Bloch method "builds-in" the finite radius BC

Standard method: solve diff. eqn. in the presence of a BC

$$[\mathscr{H} - E]\,\psi(r) = f(r), \qquad r < R$$

$$\frac{\hbar^2}{2MR}\left[\frac{d}{dr}\left(r\psi(r)\right)\right]_R = A, \qquad r = R$$

Equivalent to:

$$[\mathscr{H} - E]\,\psi(r) = F(r), \qquad F(r) = f(r) + A\delta(r - R)$$

$$\mathscr{H} = H + \mathscr{L}_0, \qquad \mathscr{L}_0 = \frac{\hbar^2}{2M}\frac{\delta(r-R)}{R}\frac{d}{dr}r$$

Representation independence of Bloch operator

- The singular Dirac delta function is only present in the position representation ('R' is the channel radius)

$$\mathscr{L}_B = \frac{\hbar^2}{2M}\frac{\delta(r-R)}{R}\left(\frac{d}{dr}r - B\right)$$

- Equivalent to

$$\hat{\mathscr{L}}_B = \frac{iR^2}{2M}|R\rangle\langle R|\left(\hat{p}_r + iB\right)$$

$$\langle r|\hat{p}_r = \frac{-i}{r}\frac{\partial}{\partial r}r\langle r|$$

- Bloch operator as a projection operator

The scattering matrix

$R = a$

- Solve Schrodinger:

$$0 = [H - E]\,|\Psi\rangle \qquad \hat{\mathscr{L}}_L|\Psi\rangle = \left[H - E + \hat{\mathscr{L}}_L\right]|\Psi\rangle$$

$$G_L\hat{\mathscr{L}}_L|\Psi\rangle = |\Psi\rangle \qquad G_L = \left[H - E + \hat{\mathscr{L}}_L\right]^{-1}$$

- Scattering BC (single channel, s-wave, neutral):

$$|\mathscr{O}\rangle = |+k\rangle \qquad |\mathscr{I}\rangle = |-k\rangle \qquad \langle r|\pm k\rangle = \frac{e^{i(\pm k)r}}{r}$$

$$\hat{\mathscr{L}}_L|+k\rangle = 0 \qquad \hat{\mathscr{L}}_L|-k\rangle = -\frac{ia^2k}{m}|a\rangle\langle a|-k\rangle$$

- Solve for the scattering matrix

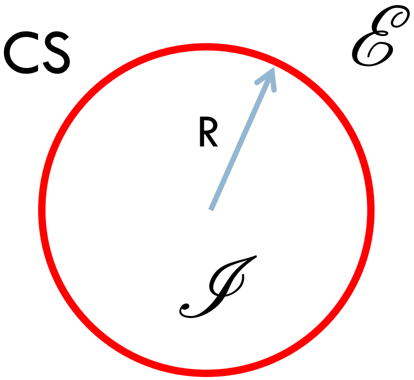
$$G_L\hat{\mathscr{L}}_L|\Psi\rangle = |\Psi\rangle$$

$$-i\frac{a^2k}{m}G_L|a\rangle\langle a|-k\rangle = |-k\rangle - S|+k\rangle$$

$$S = \frac{\langle a|-k\rangle}{\langle a|+k\rangle}\left\{1 + i\frac{a^2k}{m}\langle a|G_L|a\rangle\right\}$$

Computing $\langle a|G_L|a\rangle$ in an orthonormal basis

- Solve for Schr. eq. for general BC ("B") interior to CS



$$(H + \hat{\mathscr{L}}_B)|\lambda\rangle = E_\lambda|\lambda\rangle$$

$$\hat{\mathscr{L}}_B = \frac{ia^2}{2M}|a\rangle\langle a|\Big(\hat{p}_r + iB\Big)$$

$$B^* = B$$

$$S = \frac{\langle a|-k\rangle}{\langle a|+k\rangle}\left\{1 + i\frac{a^2k}{m}\langle a|G_L|a\rangle\right\}$$

Hard sphere

Poles, cuts

$$G_L^{-1} = H - E + \hat{\mathscr{L}}_L$$

$$\langle a|G_L^{-1}|a\rangle = \sum_{\lambda'\lambda}\langle a|\lambda'\rangle A^{-1}_{\lambda'\lambda}\langle\lambda|a\rangle \qquad A^{-1}_{\lambda'\lambda} \equiv \langle\lambda'|G_L^{-1}|\lambda\rangle$$

$$\begin{aligned}
A^{-1}_{\lambda'\lambda} &= \langle\lambda'|\Big[(H + \hat{\mathcal{L}}_B - E) + (\hat{\mathcal{L}}_L - \hat{\mathcal{L}}_B)\Big]|\lambda\rangle \\
&= (E_\lambda - E)\langle\lambda'|\lambda\rangle + i\frac{a^2}{2m}\langle\lambda'|a\rangle(iL - iB)\langle a|\lambda\rangle \\
&= (E_\lambda - E)\delta_{\lambda'\lambda} + \gamma_{\lambda'}(B - L)\gamma_\lambda \\
&= E_\lambda\delta_{\lambda'\lambda} + \Delta_{\lambda'\lambda} - i\Gamma_{\lambda'\lambda}/2 - E\delta_{\lambda'\lambda}
\end{aligned}$$

$$L \equiv S + iP$$

$$\gamma_\lambda \equiv \frac{1}{\sqrt{2m}}a\langle\lambda|a\rangle$$

$$\Delta_{\lambda'\lambda} = \gamma_{\lambda'}(B - S)\gamma_\lambda$$

$$\Gamma_{\lambda'\lambda} = \gamma_{\lambda'}(2P)\gamma_\lambda$$

Bloch/GF formalism: multichannel, charged case

- Solve Schrodinger knowing External solution (‘a’ chan. rad.)

$$[H-E]\Psi=0, \qquad [H-E+\mathscr{L}]\Psi=\mathscr{L}\Psi, \qquad \Psi=r^{-1}\Big[I-OS\Big]_{r\geq a}$$

$$\Psi=G\mathscr{L}\Psi, \qquad G=[H-E+\mathscr{L}]^{-1}, \qquad \mathscr{L}=a^{-1}\left(\rho\frac{\partial}{\partial\rho}-B\right)$$

$$I-OS=R\left(\rho\frac{\partial}{\partial\rho}-B\right)[I-OS], \qquad R\equiv G\Big|_{\mathscr{S}}, \qquad \rho\frac{\partial}{\partial\rho}O=LO$$

$$S=O^{-1}I+2i\rho O^{-1}R_L O^{-1}, \qquad R_L=\Big[1+R(B-L)\Big]^{-1}R, \qquad \rho\frac{\partial}{\partial\rho}I=LI-2i\rho O^{-1}$$

- External Coulomb wave function relations

$$O=I^*=G+iF, \qquad 1=GF'-G'F,$$

$$L=\rho O^{-1}\frac{\partial}{\partial\rho}O\equiv\mathcal{S}+iP, \qquad \mathcal{S}=\rho\frac{GG'+FF'}{G^2+F^2}, \qquad P=\rho\frac{1}{G^2+F^2}$$

Bloch/GF formalism: multichannel unitarity

$$S = O^{-1}I + 2i\rho O^{-1}R_L O^{-1}$$

$$S^\dagger = OI^{-1} - 2i\rho I^{-1}R_L^\dagger I^{-1}$$

$$\left(M^\dagger\right)^{-1} = \left(M^{-1}\right)^\dagger$$

$$S^\dagger S = 1 + 2i\rho I^{-1}R_L^\dagger\left[(R_L^{-1})^\dagger - R_L^{-1} + 2i\rho I^{-1}O^{-1}\right]R_L O^{-1}$$

$$R_L^{-1} = R^{-1} + B - L$$

$$B = B^* \implies L - L^* = 2i\rho I^{-1}O^{-1} \text{ or } P = \rho\frac{1}{G^2 + F^2}$$

$$R_{c'c} = (c'|\left[H + \mathscr{L} - E\right]^{-1}|c) = \sum_\lambda \frac{\gamma_{c'\lambda}\gamma_{c\lambda}}{E_\lambda - E}$$

- Unitarity requires B real
- Energy independent level E_λ and reduced width $\gamma_{c\lambda}$ require B constant
- Unitarity is lost if $B = \mathcal{S}(E)$ with constant E_λ, $\gamma_{c\lambda}$

Unitarity constraint on T matrix

$$\left.\begin{array}{ll}\delta_{fi} & = \sum_n S^\dagger_{fn} S_{ni} \\ S_{fi} & = \delta_{fi} + 2i\rho_f T_{fi} \\ \rho_n & = \delta(H_0 - E_n)\end{array}\right\}$$

$$T_{fi} - T^\dagger_{fi} = 2i \sum_n T^\dagger_{fn} \rho_n T_{ni}$$

NB: unitarity implies optical theorem $\sigma_{\text{tot}} = \frac{4\pi}{k} \text{Im } f(0)$; but *not just* the O.T.

- **Implications of unitarity constraint on transition matrix**
  1. Doesn't uniquely determine T_{ij}; highly restrictive, however

     Elastic: $\text{Im } T^{-1}_{11} = -\rho_1, \;\; E < E_2$ (assuming T & P invariance)

     Multichannel: $\text{Im } \mathbf{T}^{-1} = -\boldsymbol{\rho}$
  2. Unitarity violating transformations
     - cannot scale ***any*** set: $T_{ij} \to \alpha_{ij} T_{ij} \qquad \alpha_{ij} \in \mathbb{R}$
     - cannot rotate ***any*** set: $T_{ij} \to e^{i\theta_{ij}} T_{ij} \qquad \theta_{ij} \in \mathbb{R}$

     ★ consequence of linear 'LHS' $\propto$ quadratic 'RHS'
  3. Unitary parametrizations of data provide constraints that experiment may violate

     ★ *normalization*, in particular → $\text{Observable} \propto \text{KF} \;\; |T_{fi}|^2$

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Channel radius as ***regulator*** of the theory

- Simple example: single channel, s-wave, neutral

$$S = O^{-1}I + 2i\rho O^{-1}R_L O^{-1}, \qquad B = 0, \rho = ka$$

$$= e^{-2i\rho}\frac{1+i\rho R}{1-i\rho R}$$

$$\frac{\partial S}{\partial a} = 0 \implies 0 = \rho R'(\rho) + R(\rho) - \rho^2 R^2(\rho) - 1$$

$$R(\rho) = \rho^{-1}\tan\left(\rho + f(k)\right)$$

- f(k) is a familiar function – the phase shift

$$f(k) = \delta(k)$$

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Complete transition (T) matrix

- Wolfenstein formalism

$$\langle O_f \rangle = \frac{1}{\mathrm{Tr}(\rho_f)} \mathrm{Tr}(\rho_f O_f) = \frac{1}{\mathrm{Tr}(\rho_f)} \mathrm{Tr}(M \rho_i M^{\dagger} O_f),$$

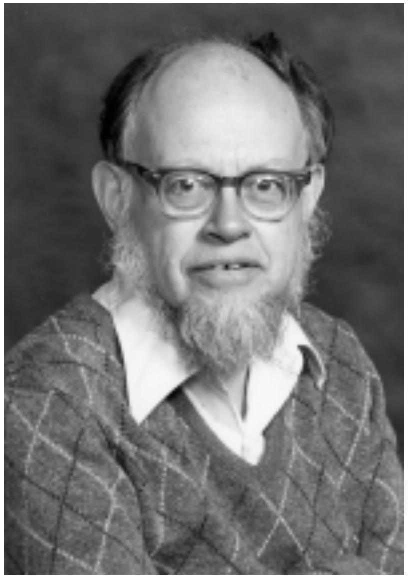
$\rho = aa^{\dagger}$, and $a_f = M a_i$.

Using the expansion $\rho_i = \frac{1}{\mathrm{Tr}(\mathbb{1}_i)} \sum_i \langle O_i \rangle \, O_i$,

and defining $\mathrm{Tr}(\rho_f) = \sigma_0(\theta)$ gives finally

$$\sigma_0(\theta) \langle O_f \rangle = \frac{1}{\mathrm{Tr}(\mathbb{1}_i)} \sum_i \langle O_i \rangle \mathrm{Tr}(M O_i M^{\dagger} O_f), \qquad \begin{cases} O_i = O_1 \otimes O_2 \\ O_f = O_3 \otimes O_4 \end{cases}$$

$$M_{fi} = \frac{4\pi}{k_i} \langle \phi_{s'}^{\mu'} | \hat{T} | \phi_s^{\mu} \rangle = \frac{4\pi}{k_i} \sum_{JMl'l} \langle \phi_{s'}^{\mu'} | \mathcal{Y}_{Js'l'}^{M} \rangle T_{s'l',sl}^{J} \langle \mathcal{Y}_{Jsl}^{M} | \phi_s^{\mu} \rangle.$$



Lincoln Wolfenstein
1923-2015

Relativistic forms of EDA

$$R = \sum_\lambda \frac{\gamma_\lambda \gamma_\lambda^T}{E_\lambda(s) - E(s)},$$

$$s = (p_1 + p_2)^2 = (p_3 + p_4)^2 = (\varepsilon_{\text{rel}} + M)^2.$$

Forms for $E_{(\lambda)}(s)$:

a) $\sqrt{s} - M = \varepsilon_{\text{rel}}$

b) $\dfrac{s - M^2}{2M} = \left(1 + \dfrac{\varepsilon_{\text{rel}}}{2M}\right)\varepsilon_{\text{rel}}$

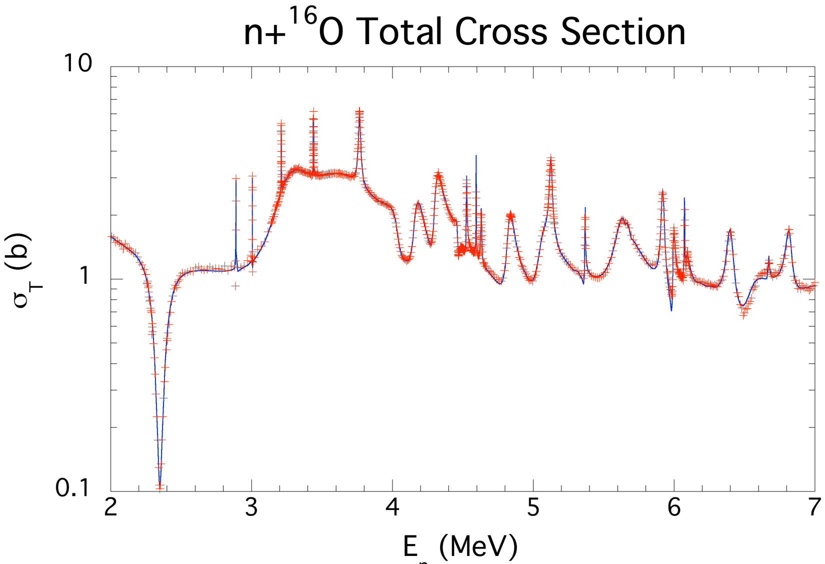
c) $\dfrac{(s - M^2)(s - \Delta^2)}{8s\mu}$ (Layson)

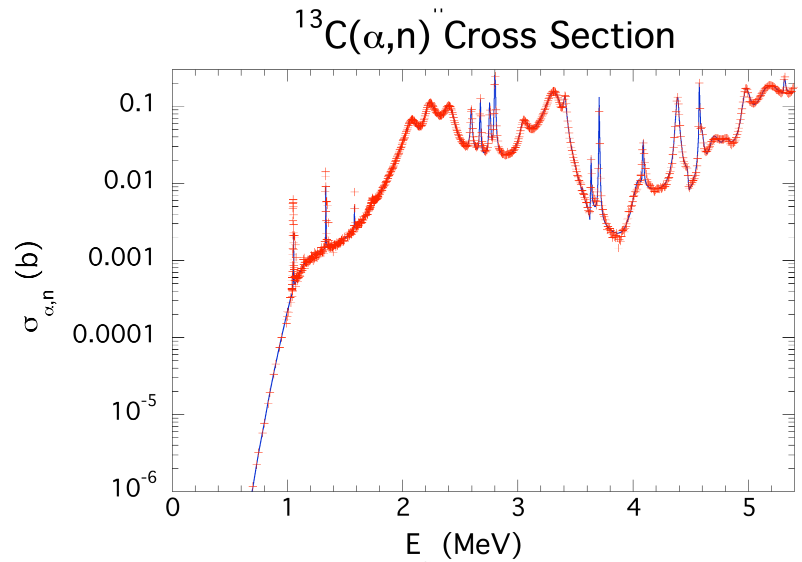
d) ε_{nr} (norel=1)

$$\begin{cases} M = m_1 + m_2 \\ \Delta = m_1 - m_2 \\ \mu = \dfrac{m_1 m_2}{m_1 + m_2} \end{cases}$$

Relativistic form: not a luxury

Here is an example from the ^{17}O system: There is a narrow $3/2^{+}$ resonance at $E_n = 3.0071$ MeV having a c.m width of 0.33 keV. Relativistically, this resonance would show up at a laboratory α-energy of $E_\alpha = 0.802717$ MeV. Non-relativistically, it would be at 0.803041 MeV. So, the difference is 0.324 keV, or 0.248 keV in the c.m., which is a significant fraction of the width of this resonance.





EM Transitions and Photon Channels

Assume that in the one-photon sector of Fock space, a "wave function" is associated with the vector potential

$$\mathbf{A}_{\mathbf{k}}(\mathbf{r}) = \sqrt{\frac{2}{\pi\hbar c}} \sum_{jm} i^j \left[\alpha_{jm}^{(e)} \mathbf{A}_{jm}^{(e)}(\mathbf{r}) + \alpha_{jm}^{(m)} \mathbf{A}_{jm}^{(m)}(\mathbf{r}) \right],$$

$$\mathbf{A}_{jm}^{(e)}(\mathbf{r}) = \frac{1}{r}\left[u_{ee}^{j}(\underbrace{\rho}_{kr}) \mathbf{Y}_{jm}^{(e)}(\hat{\mathbf{r}}) + u_{0e}^{j}(\rho) \mathbf{Y}_{jm}^{(0)}(\hat{\mathbf{r}}) \right], \text{ parity=}(-1)^j,$$

$$\mathbf{A}_{jm}^{(m)}(\mathbf{r}) = \frac{1}{r} u_{mm}^{j}(\rho) \mathbf{Y}_{jm}^{(m)}(\hat{\mathbf{r}}), \text{ parity=}(-1)^{j+1}.$$

The physical radial functions have the asymptotic forms

$$u_{ii}^{j}(\rho) = F_j^{(i)} + O_j^{(i)} t_{ii}^{j} \quad (i = e, m),$$

with $O_j^{(m)} = h_j^{+}(\rho)$, $O_j^{(e)} = -\partial_\rho h_j^{+}(\rho)$, and $F_j^{(i)} = \operatorname{Im} O_j^{(i)}$.

In the usual approach, $O_j^{(e)} = O_j^{(m)} = h_j^{+}(\rho)$.

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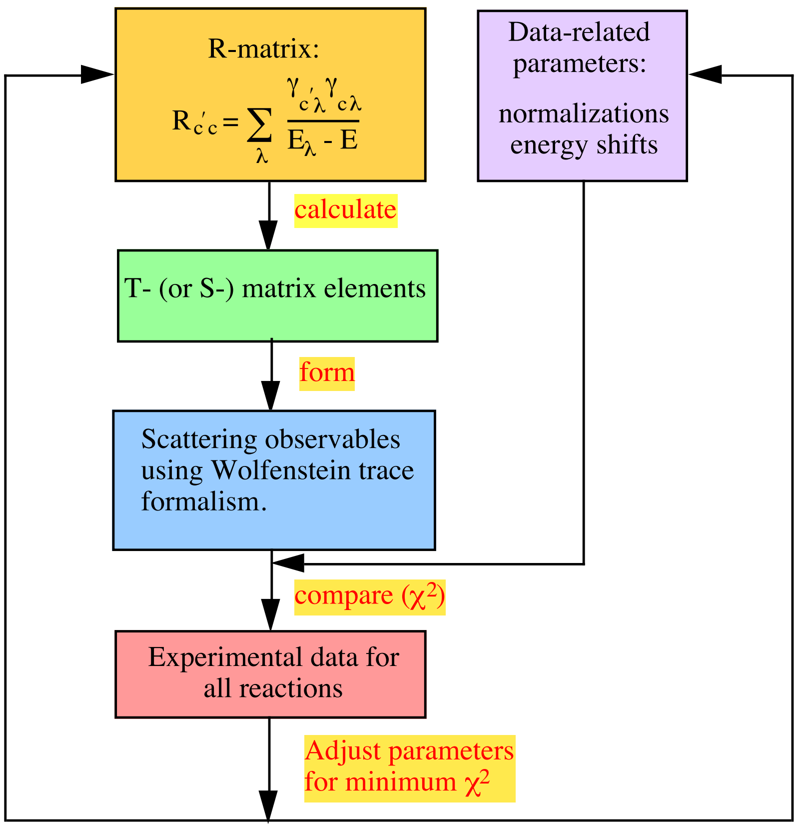
Scheme and Properties of the EDA Code

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

Uncertainties from Chi-Squared Minimization

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

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

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

The parameter covariance matrix is $\mathbf{C}_0 = 2\mathbf{G}_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\begin{aligned}\mathrm{cov}[\sigma_{\mathrm{i}}(E)\sigma_j(E')] &= \left[\nabla_{\mathbf{p}}\sigma_{\mathrm{i}}(E)\right]^{\mathrm{T}}\mathbf{C}_0\left[\nabla_{\mathbf{p}}\sigma_{\mathrm{j}}(E')\right]\Big|_{\mathbf{p}=\mathbf{p}_0} \\ &= \Delta\sigma_{\mathrm{i}}(E)\Delta\sigma_{\mathrm{j}}(E')\rho_{ij}(E,E').\end{aligned}$$

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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

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

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

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

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), $\Delta\chi^2_{\max} \approx k = \left\langle\Delta\chi^2\right\rangle$. This results in 1-σ parameter confidence intervals,*

$$\Delta p_i \le \sqrt{2\Delta\chi^2_{\max}H_{ii}} = \sqrt{\Delta\chi^2_{\max}C^0_{ii}} \approx \sqrt{kC^0_{ii}},$$

that are $\sim\sqrt{k}$ larger than the standard deviations (σ_{p_i}).

* when the remaining parameters are adjusted to obtain a new chi-square minimum

^{7}Li system analysis

Channel	a_c (fm)	l_{max}
t+^{4}He	4.02	5
n+^{6}Li	5.0	3
n+^{6}Li*	5.5	1
d+^{5}He	6.0	0

$$\chi^2_{\text{EDA}} = \sum_i \left[\frac{nX_i(\mathbf{p}) - R_i}{\Delta R_i}\right]^2 + \left[\frac{nS-1}{\Delta S/S}\right]^2,$$

Reaction	Energy Range	# Pts.	Observables
^{4}He(t,t)^{4}He	E_t=0 - 14	1661	$\sigma(\theta)$, $A_y(t)$
^{4}He(t,n)^{6}Li	E_t = 8.75 - 14.4	37	σ_{int}, $\sigma(\theta)$
^{4}He(t,n)^{6}Li*	E_t =12.9	4	$\sigma(\theta)$
^{6}Li(n,t)^{4}He	E_n = 0 - 4	1406	σ_{int}, $\sigma(\theta)$
^{6}Li(n,n)^{6}Li	E_n = 0 - 4	800	σ_T, σ_{int}, $\sigma(\theta)$, $P_y(n)$
^{6}Li(n,n')^{6}Li*	E_n = 3.35 - 4	8	σ_{int}
^{6}Li(n,d)^{5}He	E_n = 3.35 - 4	2	σ_{int}
Total		3918	13

The EDA **R**-matrix analysis included data for all reactions open in the ^{7}Li system at energies up to E_n = 4 MeV (E_x=10.7 MeV). The data set, which included more than 3900 experimental points, is summarized in Table I. The χ^2 per degree of freedom for the analysis is 1.36. The original experimental uncertainties were not changed, but outlier points having χ^2 > 10 were discarded from the fit.

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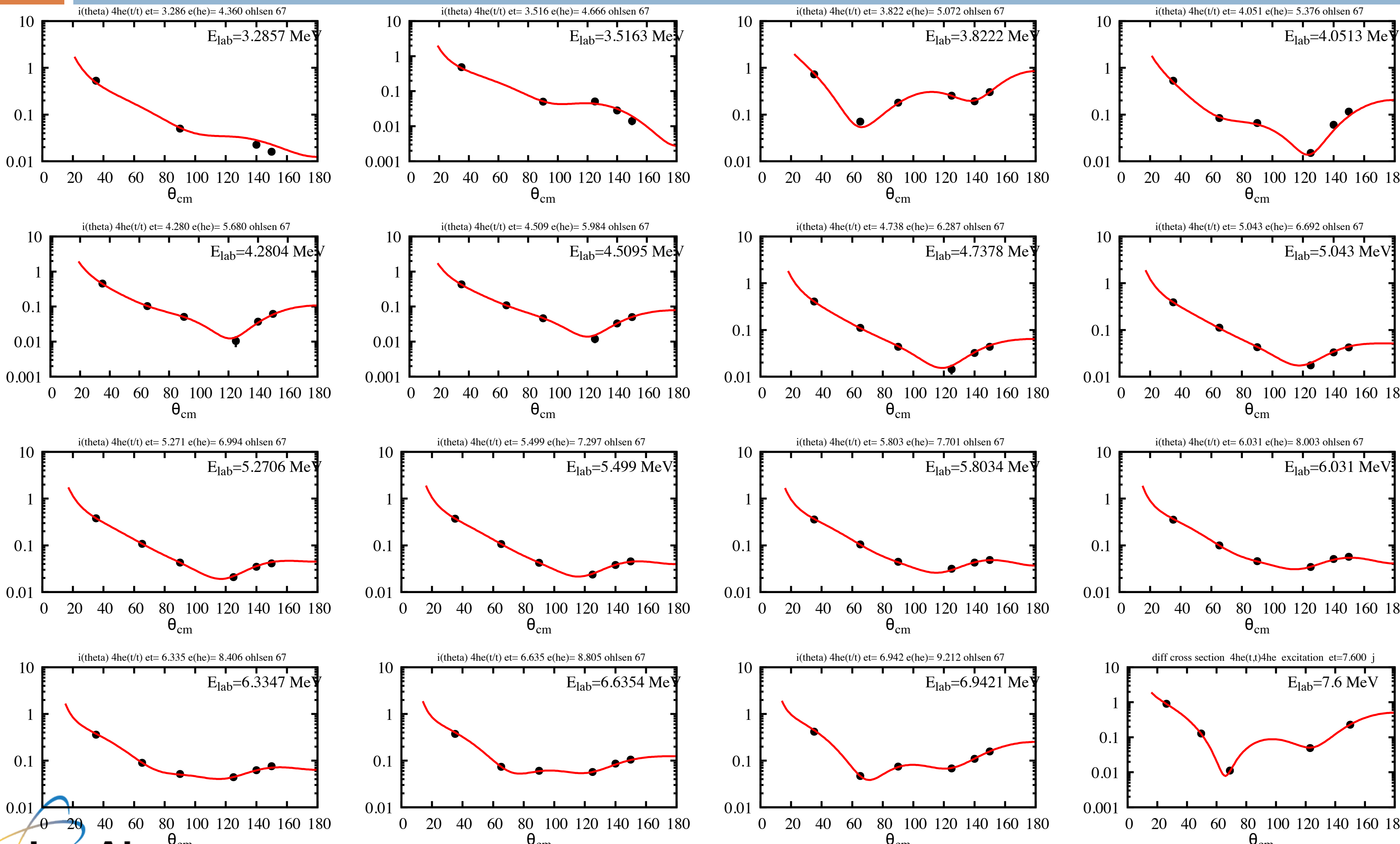
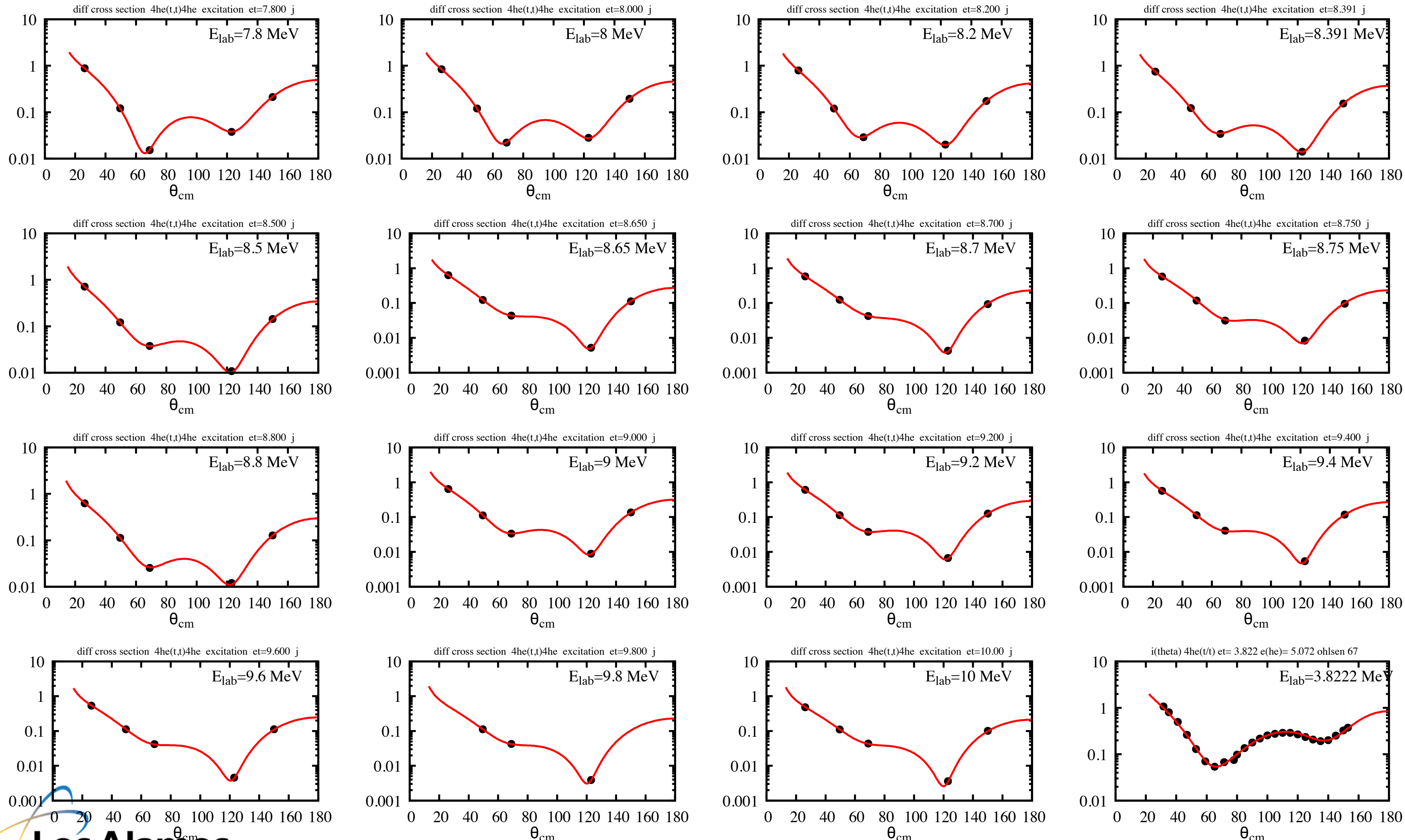
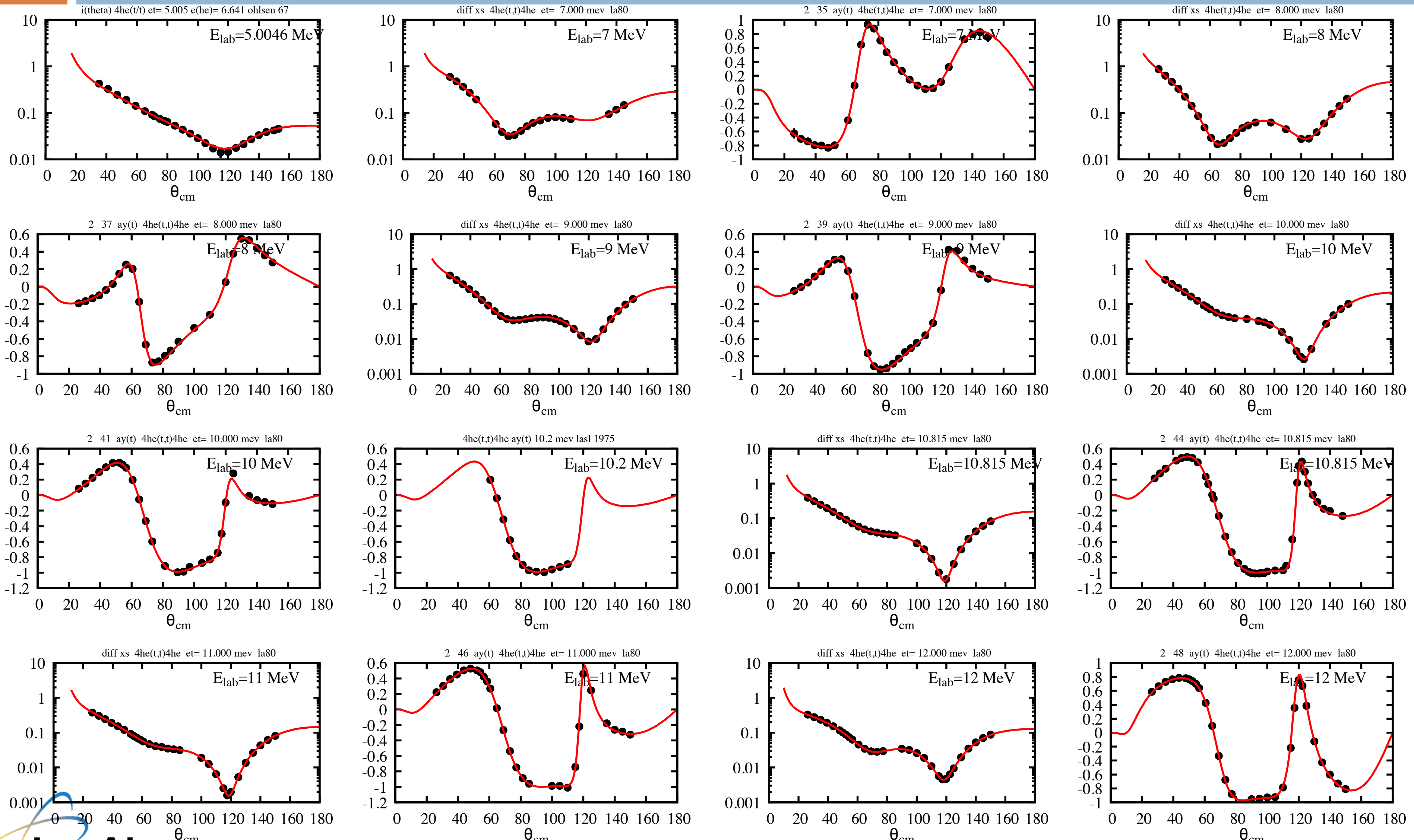
Angular distributions: ^{4}He(t,t) DCS



Angular distributions: $^4He(t,t)$ DCS



Angular distributions: ^{4}He(t,t) DCS & A_y



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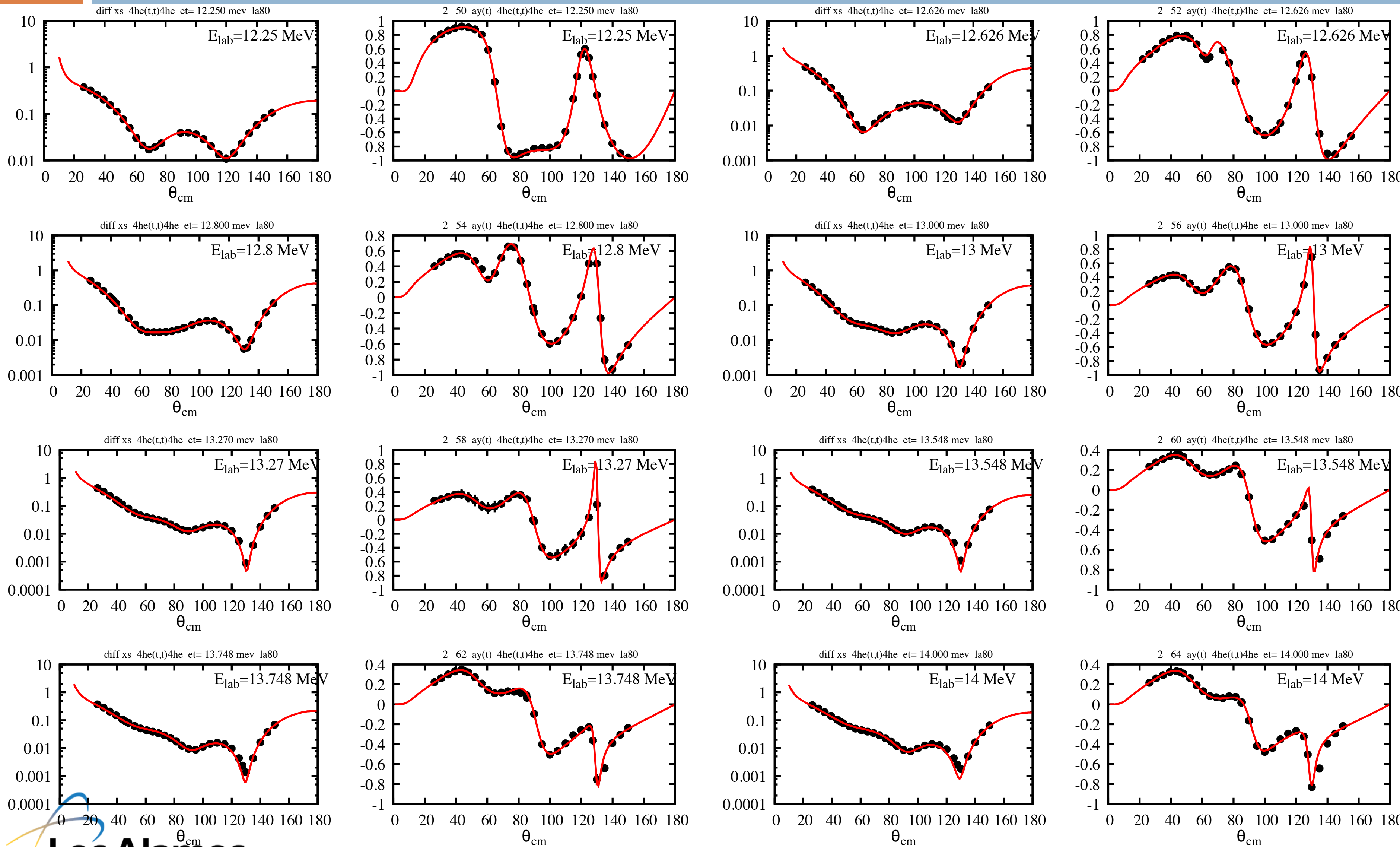
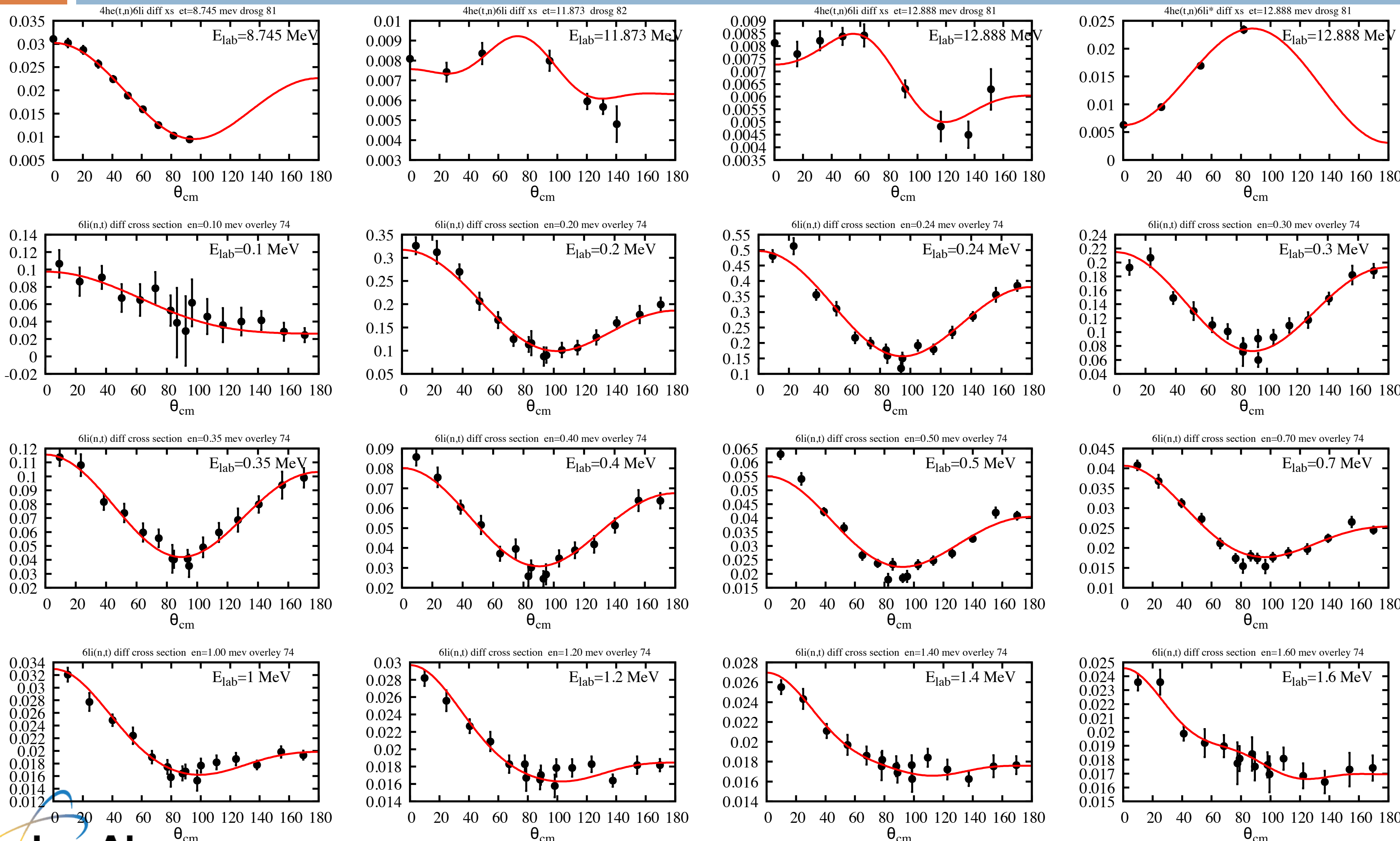
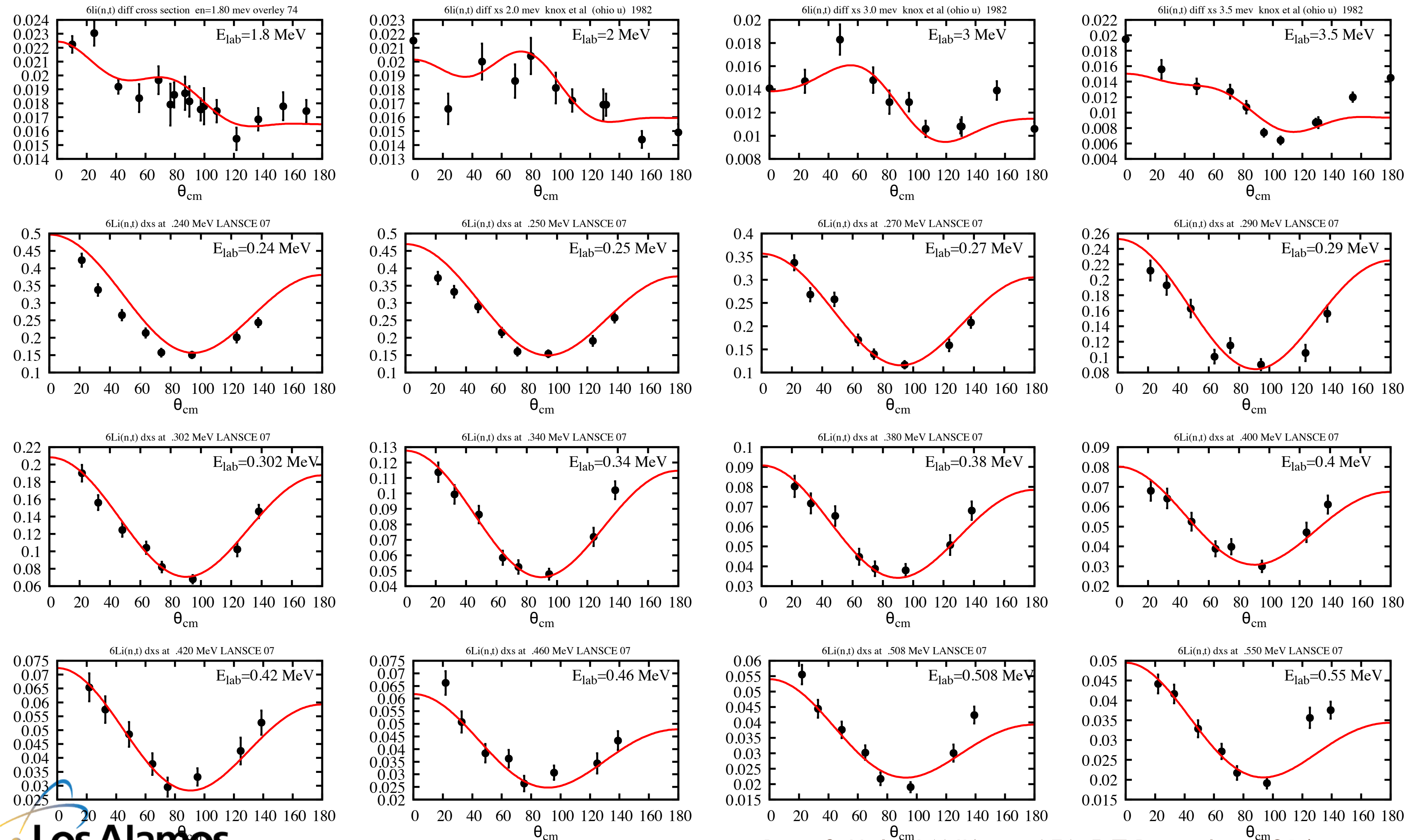
Angular distributions: $^4He(t,t)$ DCS & A_y



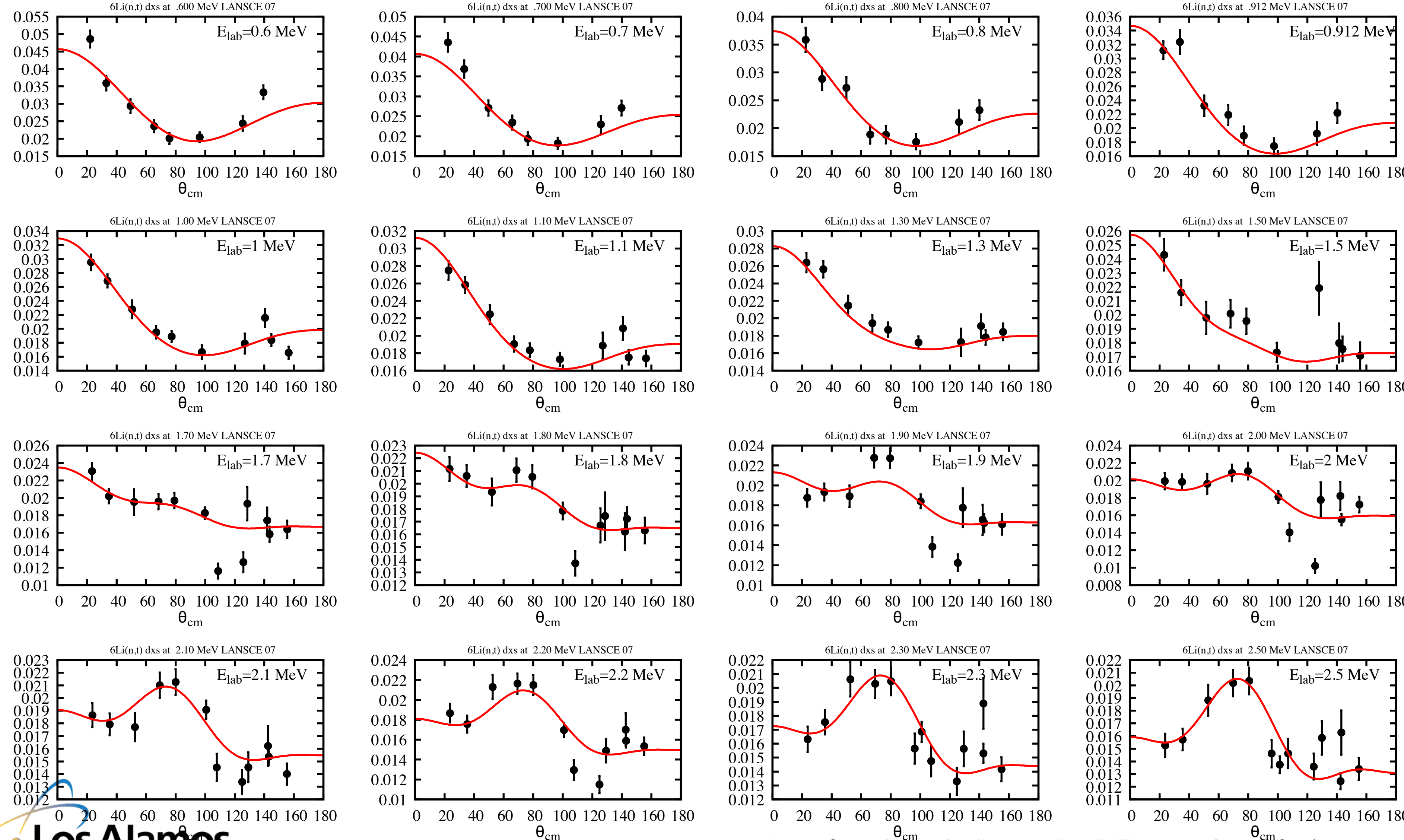
Angular distributions: ^{4}He(t,n) & ^{6}Li(n,t) DCS



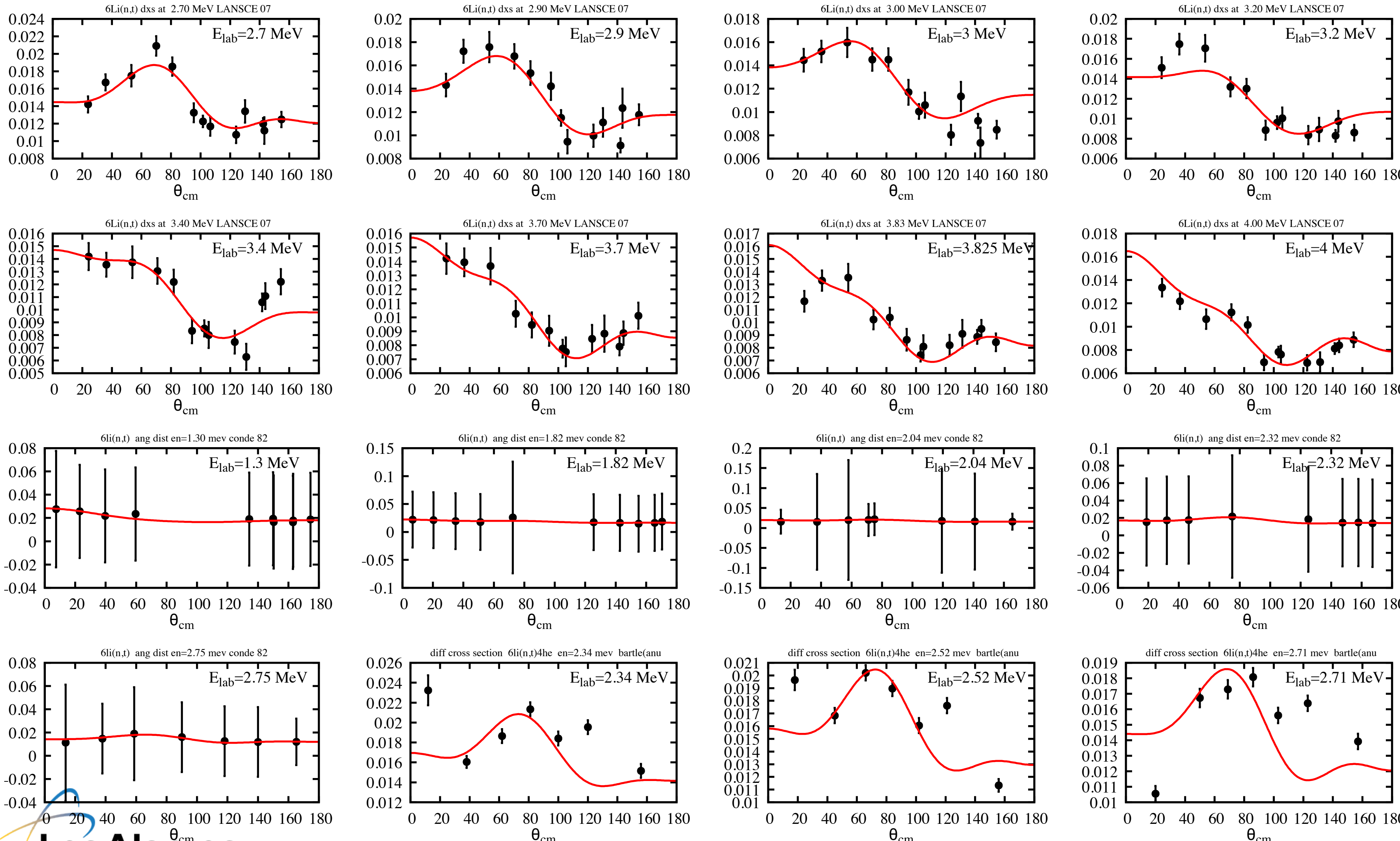
Angular distributions: ^{6}Li(n,t) DCS



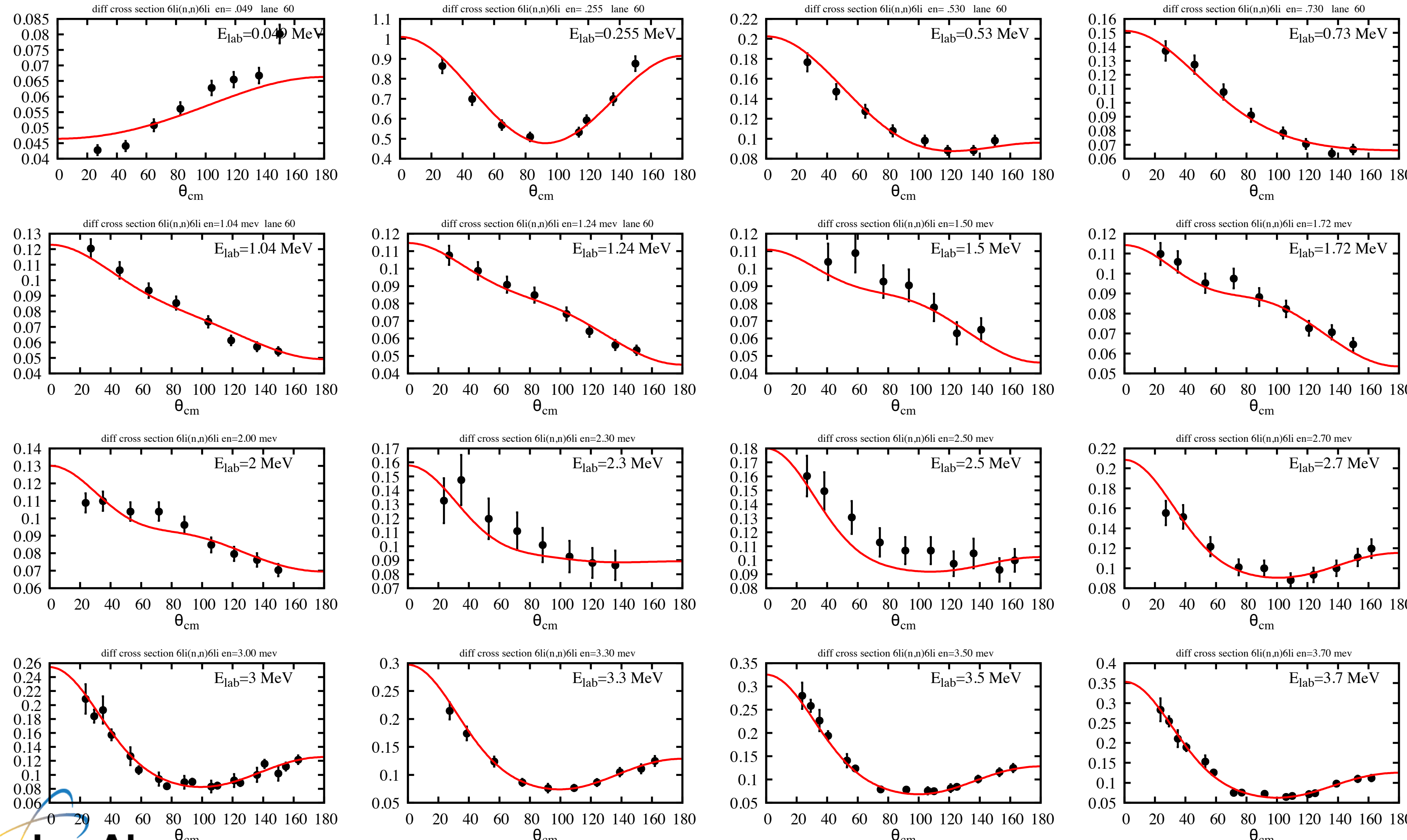
Angular distributions: ^{6}Li(n,t) DCS



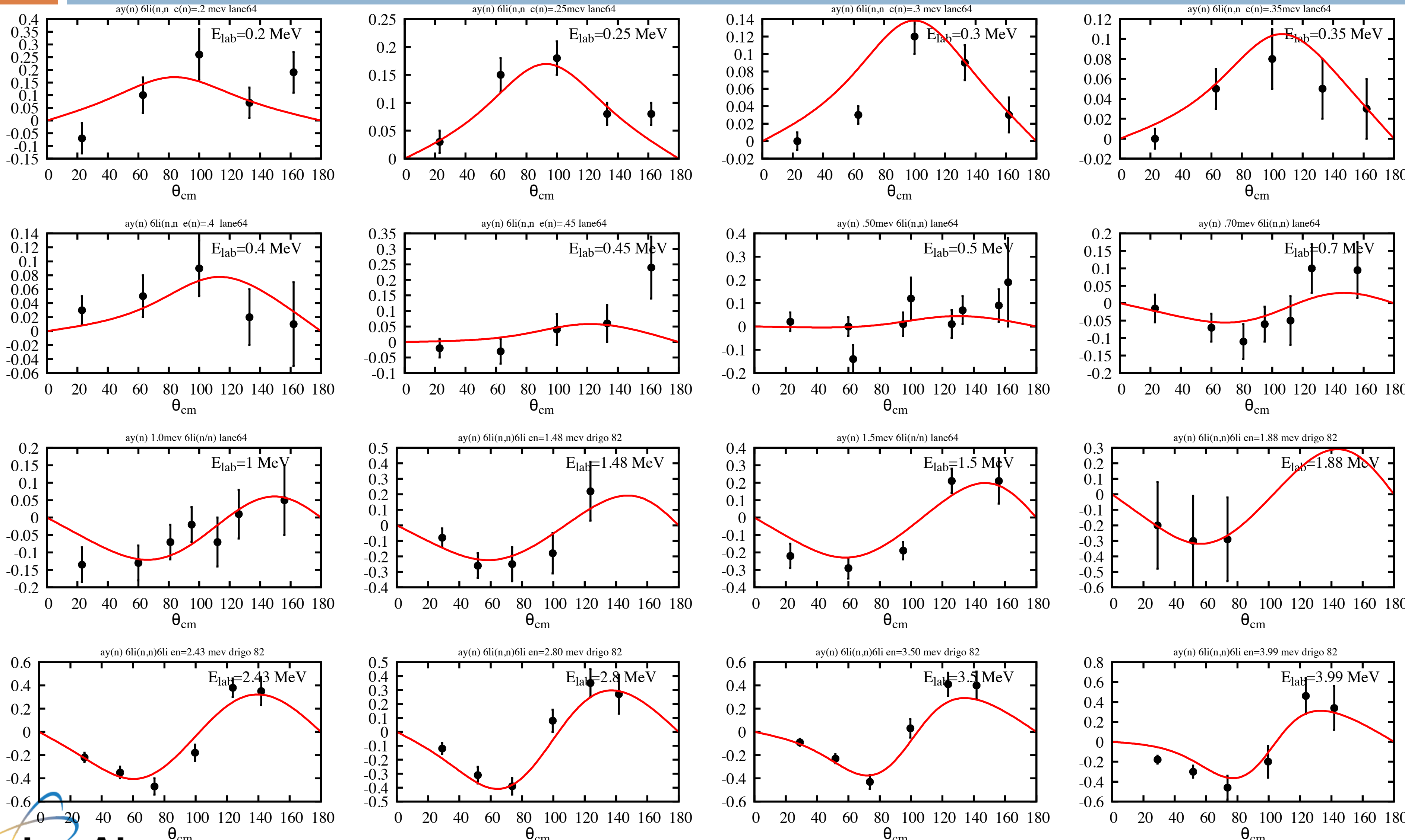
Angular distributions: ^{6}Li(n,t) DCS



Angular distributions: ^{6}Li(n,n) DCS



Angular distributions: $^6Li(n,n)\ A_y$



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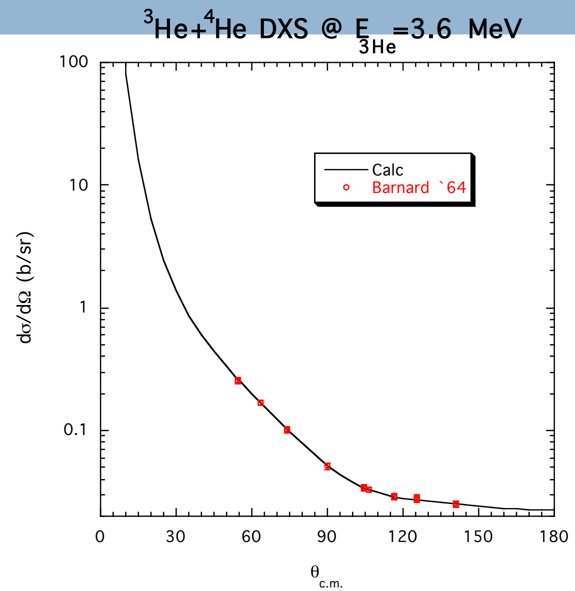
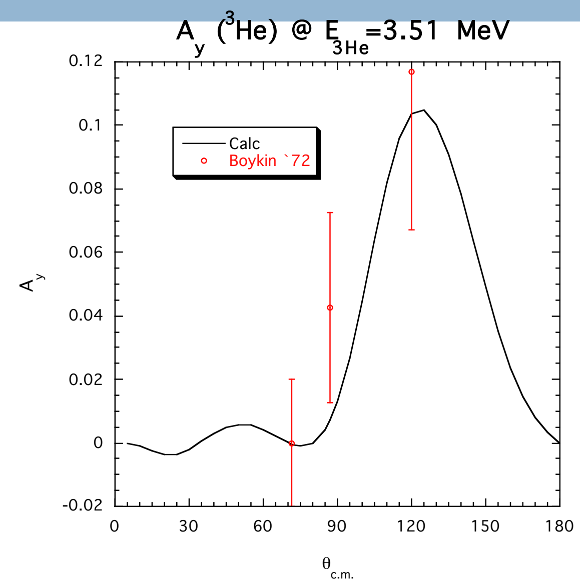
^{7}Be System Analysis

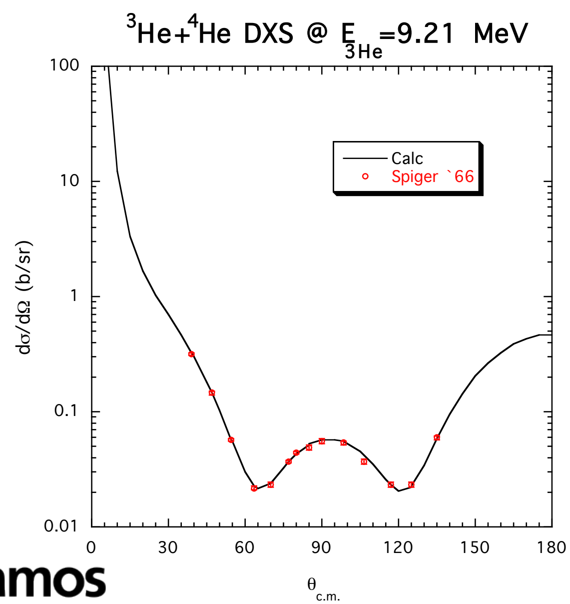
Channel	l_{max}	a_c (fm)
^{3}He+^{4}He	4	4.4
p+^{6}Li	1	3.1
γ+^{7}Be	1	50

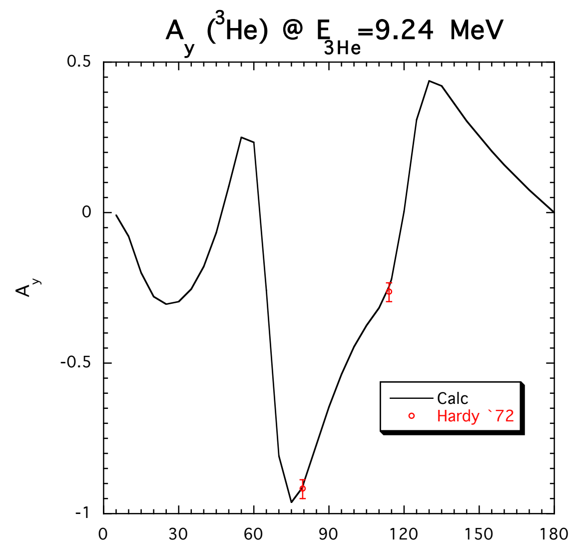
Reaction	Energy range (MeV)	# obs. types	# data points
^{4}He(^{3}He,^{3}He)^{4}He	E_{3He} = 1.7-10.8	2	1487
^{4}He(^{3}He,p)^{6}Li	E_{3He} = 8.2-10.8	1	130
^{4}He(^{3}He,γ)^{7}Be	E_{3He} = 0-2.2	1	40
^{6}Li(p, ^{3}He)^{4}He	E_p = 0-2.7	2	488
^{6}Li(p,p)^{6}Li	E_p = 1.2-2.5	1	187
^{6}Li(p,γ)^{7}Be	E_p = 0-1.2	1	28
Totals		8	2360

Example: ^{3}He+^{4}He Scattering

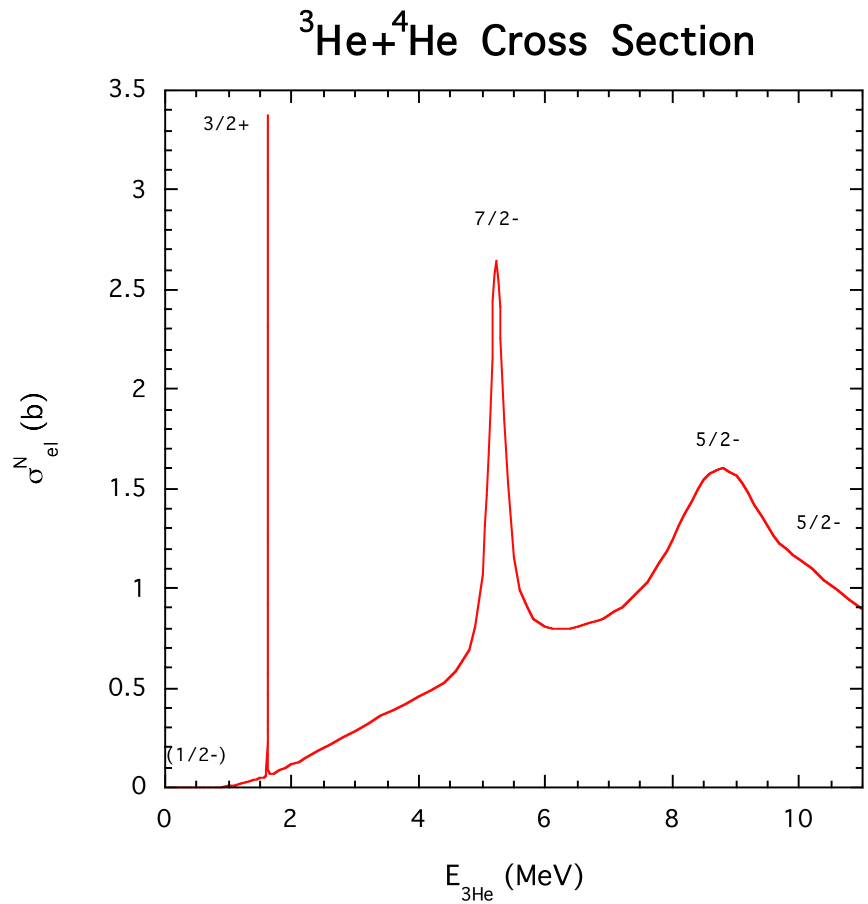


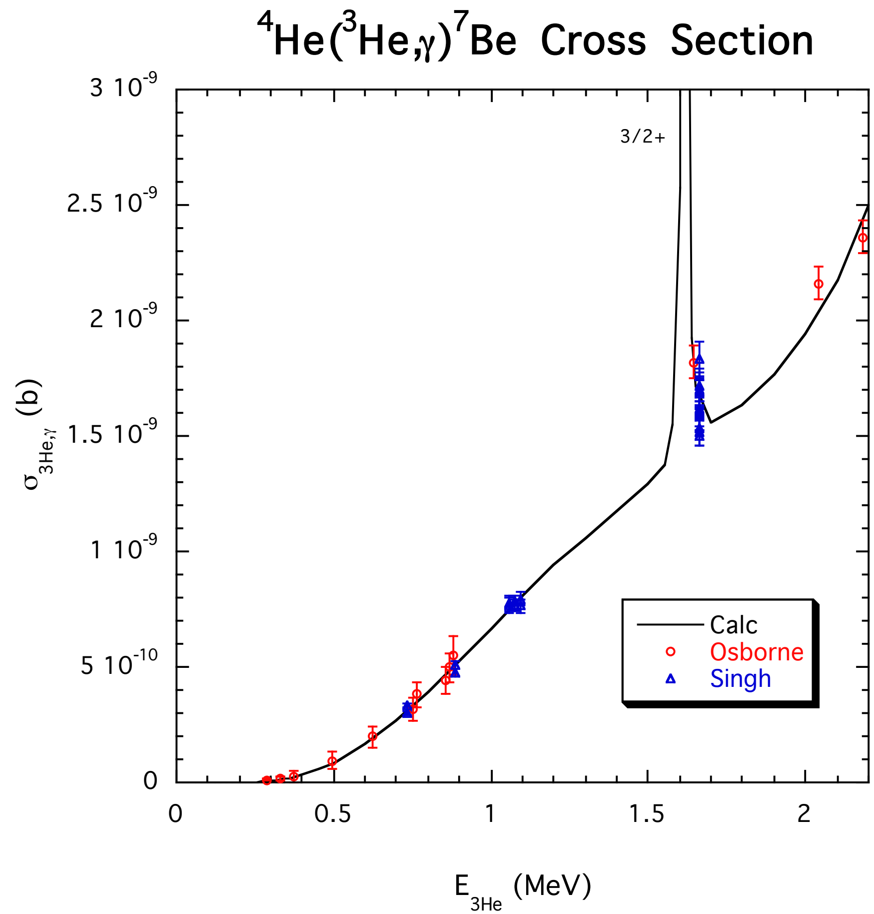






Resonances in the Cross Sections





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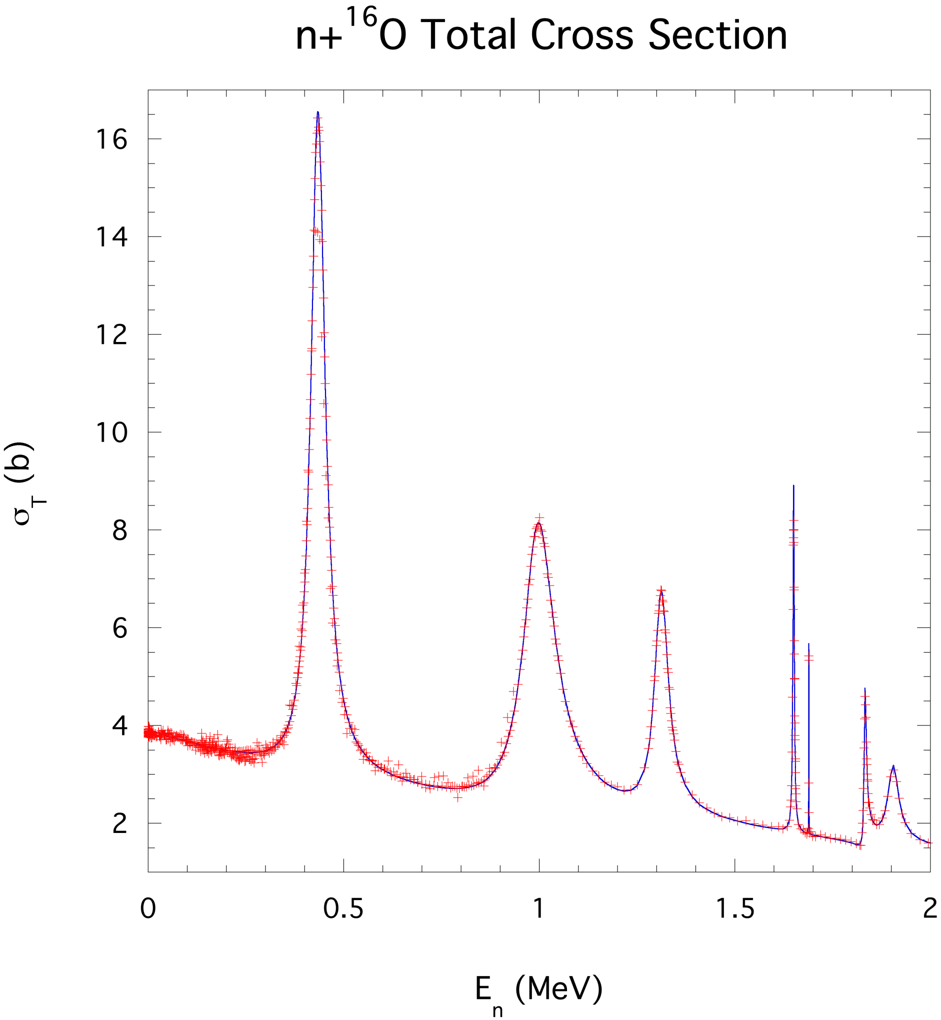
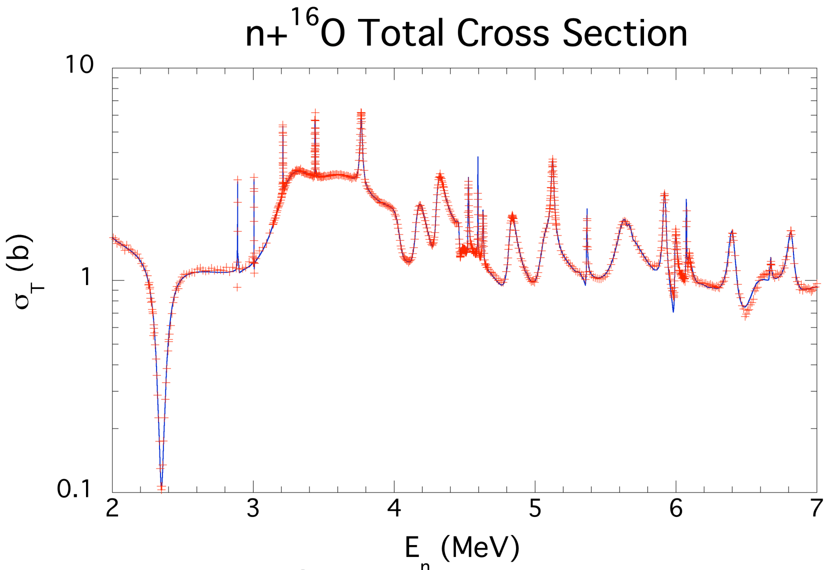
^{17}O System Analysis

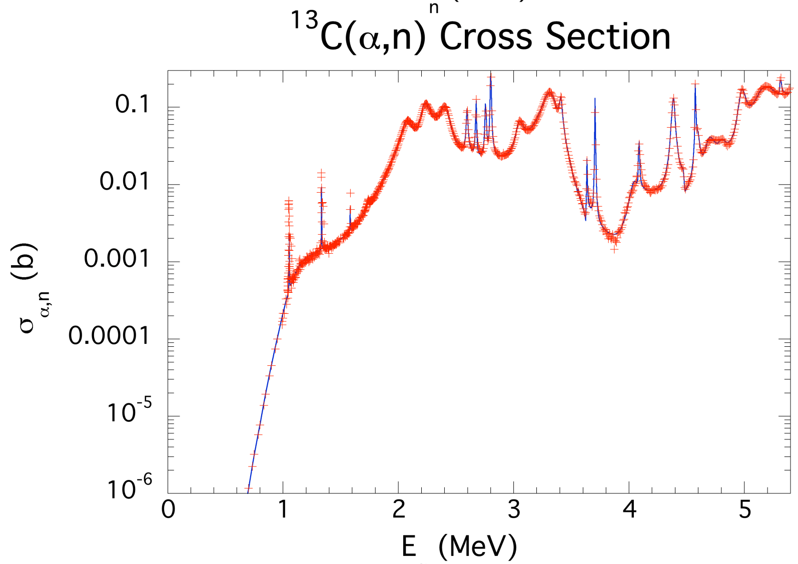
Channel	a_c (fm)	l_{max}
$n+^{16}O$	4.3	4
$\alpha+^{13}C$	5.4	5

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

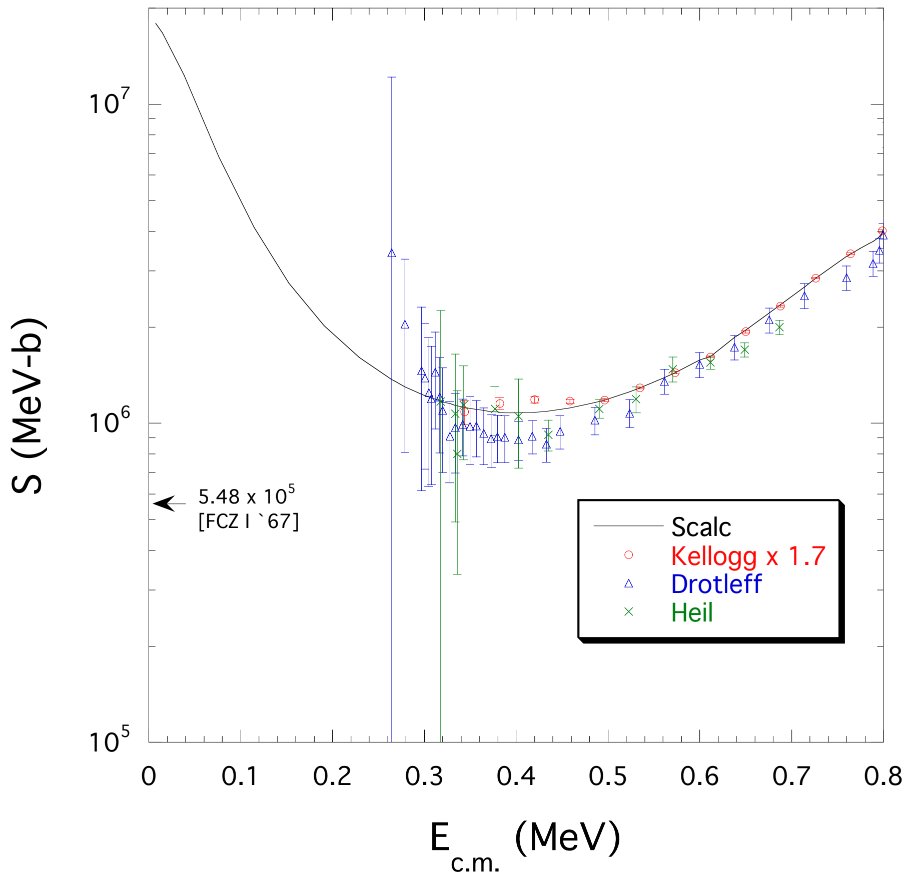
^{17}O System: comparison with data



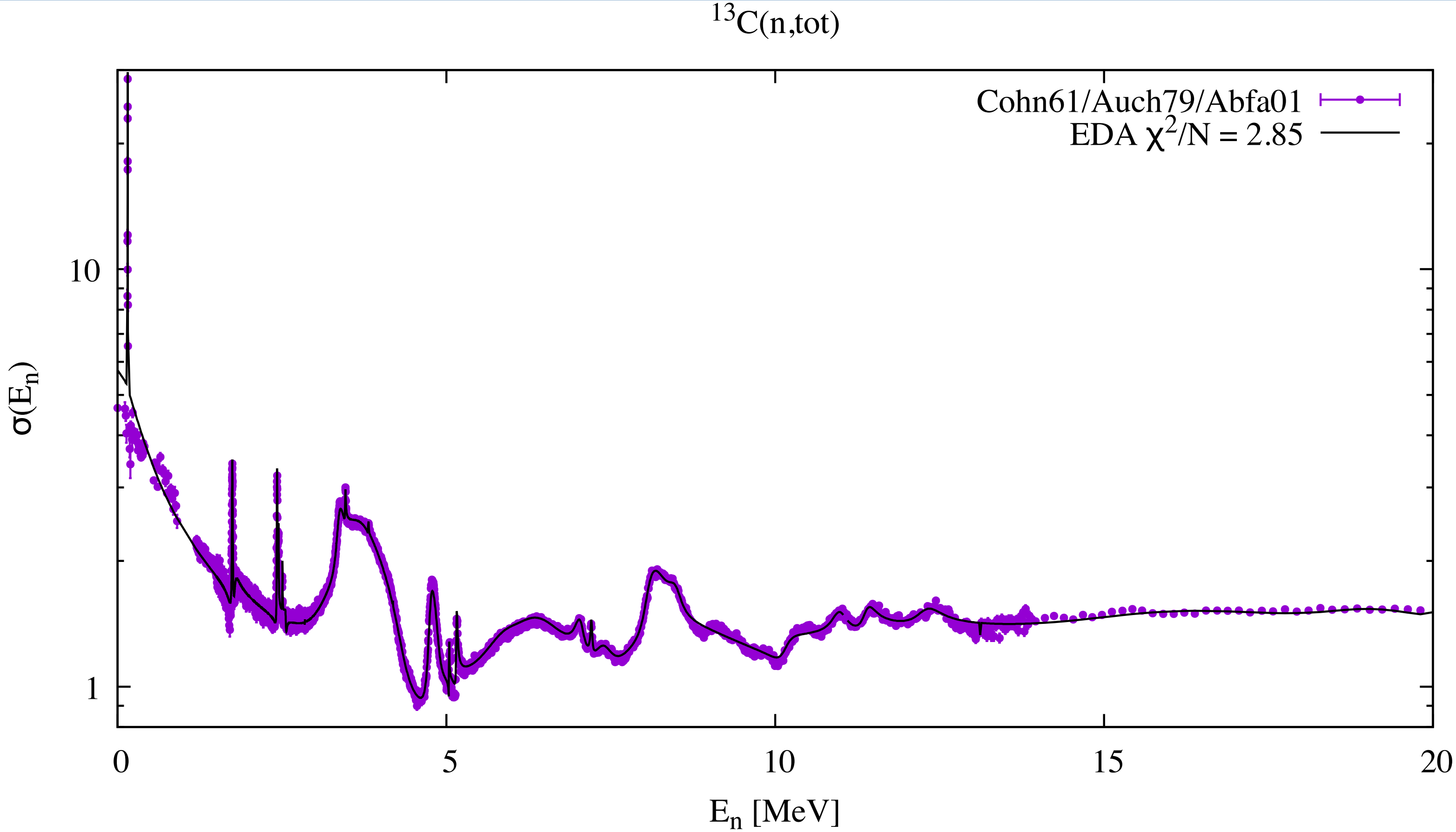




^{17}O System: $^{13}C(a,n)^{16}O$ S-factor



Recent development in EDA5 capability



- R-matrix fit to 20 MeV: 6 partitions; 93 channels; largest analysis
- $n^{13}C, n_1{}^{13}C^*, n_2{}^{13}C^*, \alpha^{10}Be, n_3{}^{13}C^*, nn^{12}C$

EDA6: modern Fortran implementation

- Improved physics capabilities
  - Enlarge channel space to extend energy range to >20 MeV
  - Hyperspherical approach to multiparticle break-up (total x-sec.)
- Data handling
  - Automated/integrated with CSISRS/EXFOR c4/c5 format
  - Data covariance standardization
- Fitting
  - Data covariance
  - Bayesian event-based maximum likelihood approach
- Exchange
  - ENDF-6 format/ACE/NDI/…
  - Resonance parameters: Brune alternative; ***T-matrix poles***

Brune parameters vs. T-matrix poles

- The Brune parameters are useful for exchange purposes

$$\mathcal{E} = e - \sum_c \gamma_c \gamma_c^T (S_c - B_c) \qquad \mathcal{E} a_i = \tilde{E}_i a_i$$

  - ***But they depend on the channel radii; <u>EDA & AMUR allow these to float</u>***
- As a check of the observable equivalence of various analyses, finding the poles of the T-matrix isn't much more difficult

$$\det A(E)\Big|_{E=\{E_R\}} = 0 \qquad A^{-1}_{\lambda'\lambda} = E_\lambda \delta_{\lambda'\lambda} + \Delta_{\lambda'\lambda} - i\Gamma_{\lambda'\lambda} - E\delta_{\lambda'\lambda}$$

- ENDF-6 format
  - Brune parameters (LRP=1, LRF=7): can be used to compute observables
  - T-matrix poles (LRP=2, LRF=7): are used for analysis comparisons