

R-MATRIX METHODS & APPLICATIONS WITH **EDA**

Outline

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- Overview
 - History at LANL
 - Existing analyses
- R-matrix formalism
 - Bloch formalism
 - Wolfenstein formalism
 - Fitting, errors, covariance
- Analyses (systems)
 - ${}^7\text{Be}$, ${}^{17}\text{O}$
- Resonance model (if there's time)
 - Particle spectra

Overview of multichannel reaction analysis

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- History of **E**nergy **D**ependent **A**nalysis
 - Developers: D. Dodder, K. Witte, G. Hale, A. Sierk, MP
 - Some original motivation: hadronic analyses e.g. $\pi N \rightarrow \pi N$
 - EDA5 F77; EDA6 F90/95 (under development)
- Code 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

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

EDA Existing Analyses, Cont.

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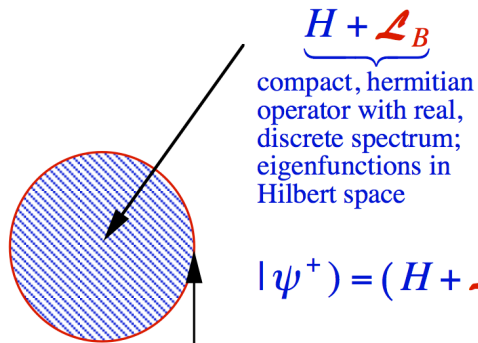
A	System (Channels)
6	${}^6\text{He}$ (${}^5\text{He}+n$, $t+t$); ${}^6\text{Li}$ ($d+{}^4\text{He}$, $t+{}^3\text{He}$); ${}^6\text{Be}$ (${}^5\text{Li}+p$, ${}^3\text{He}+{}^3\text{He}$)
7	${}^7\text{Li}$ ($t+{}^4\text{He}$, $n+{}^6\text{Li}$); ${}^7\text{Be}$ ($\gamma+{}^7\text{Be}$, ${}^3\text{He}+{}^4\text{He}$,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

2→2 body R matrix formalism

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\mathcal{I}

INTERIOR (Many-Body) REGION
(Microscopic Calculations)



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

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

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

SURFACE

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

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

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

\mathcal{E}

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

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

or equivalently,

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

Measurements

Bloch/Green-function formalism: Hermiticity

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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

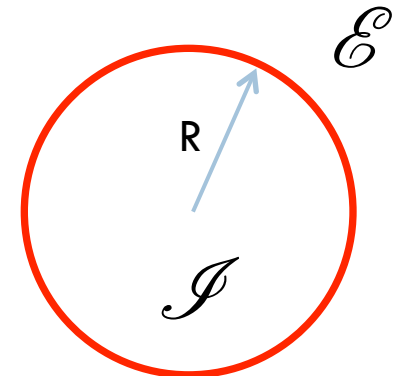
Claude Bloch¹

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

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

$$\mathcal{H} = H + \frac{\hbar^2}{2MR} \delta(r - R) \frac{d}{dr} r,$$

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



Bloch/GF formalism: Generalized GF

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$$[\mathcal{H} - E] \psi(r) = F(r),$$

$$\mathcal{H} = H + \mathcal{L}_0,$$

$$F(r) = f(r) + A\delta(r - R)$$

$$\mathcal{L}_0 = \frac{\hbar^2}{2M} \frac{\delta(r - R)}{R} \frac{d}{dr} r$$

Equivalent to:

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

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

Bloch/GF formalism: representation independence

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

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

- Equivalent to

$$\hat{\mathcal{L}}_B = \frac{\hbar^2 R^2}{2M} |R\rangle \langle R| \left(i\hat{p}_r - B \right)$$

- Bloch operator as a projection operator

Bloch/GF formalism: multichannel case

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

$$[H - E]\Psi = 0, \quad \Psi = r^{-1} [I - OS], \quad r \geq a$$

$$\Psi = G\mathcal{L}\Psi,$$

$$G = [H - E + \mathcal{L}]^{-1},$$

$$\mathcal{L} = a^{-1} \left(\rho \frac{\partial}{\partial \rho} - B \right)$$

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

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

- External Coulomb wave function relations

$$O = I^* = G + iF,$$

$$1 = GF' - G'F,$$

$$L = \rho O^{-1} \frac{\partial}{\partial \rho} O \equiv S + iP,$$

$$S = \rho \frac{GG' + FF'}{G^2 + F^2},$$

$$P = \rho \frac{1}{G^2 + F^2}$$

Bloch/GF formalism: multichannel unitarity

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

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

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

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

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

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

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

- 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 $E_{\lambda}, \gamma_{c\lambda}$

Unitarity constraint on T matrix

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

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

- Doesn't uniquely determine T_{ij} ; highly restrictive, however
Elastic: $\text{Im } T_{11}^{-1} = -\rho_1$, $E < E_2$ (assuming T & P invariance)
Multichannel: $\text{Im } \mathbf{T}^{-1} = -\rho$

2. Unitarity violating transformations

- cannot scale **any** set: $T_{ij} \rightarrow \alpha_{ij} T_{ij}$ $\alpha_{ij} \in \mathbb{R}$
- cannot rotate **any** set: $T_{ij} \rightarrow e^{i\theta_{ij}} T_{ij}$ $\theta_{ij} \in \mathbb{R}$

★ consequence of linear 'LHS' \propto quadratic 'RHS'

3. Unitary parametrizations of data provide constraints that experiment may violate

★ *normalization*, in particular

Observable \propto KF $|T_{fi}|^2$

Channel radius as *regulator* of the theory

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

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

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

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

- $f(k)$ is a familiar function – What is it?

- A request: Does anyone have Teichmann's thesis?

- Quoted in Lane & Thomas footnote #48, p. 275

Complete, polarization transition matrix

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□ Wolfenstein formalism

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

$$\rho = aa^\dagger, \text{ and } a_f = Ma_i.$$

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

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

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

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



Lincoln Wolfenstein
1923-2015

Relativistic forms of EDA

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

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

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

a) $\sqrt{s} - M = \mathcal{E}_{\text{rel}}$

b) $\frac{s - M^2}{2M} = \left(1 + \frac{\mathcal{E}_{\text{rel}}}{2M}\right) \mathcal{E}_{\text{rel}}$

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

d) \mathcal{E}_{nr} (norel=1)

$$\left\{ \begin{array}{l} M = m_1 + m_2 \\ \Delta = m_1 - m_2 \\ \mu = \frac{m_1 m_2}{m_1 + m_2} \end{array} \right.$$

EM Transitions and Photon Channels

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

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

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

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

The physical radial functions have the asymptotic forms

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

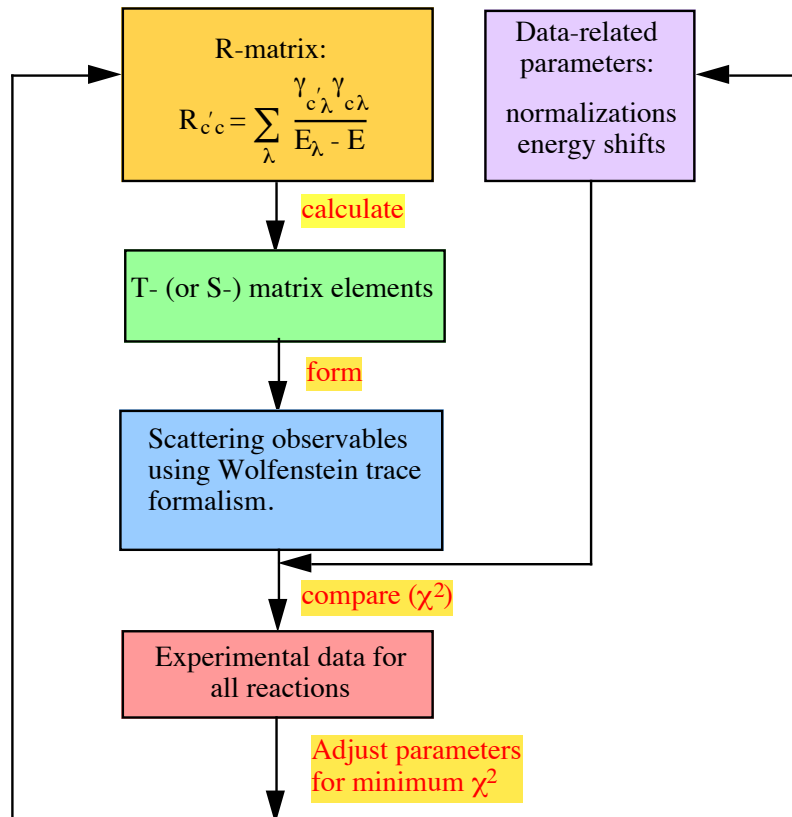
$$\text{with } O_j^{(m)} = h_j^+(\rho), \quad O_j^{(e)} = -\partial_\rho h_j^+(\rho), \quad \text{and } F_j^{(i)} = \text{Im } O_j^{(i)}.$$

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

Scheme and Properties of the EDA Code

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Energy Dependent Analysis Code



- Accommodates general (spins, masses, charges) two-body channels
- Uses relativistic kinematics and R-matrix formulation
- Calculates general scattering observables for $2 \rightarrow 2$ 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

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

$$\left\{ \begin{array}{l} R_i, \Delta R_i = \text{relative measurement, uncertainty} \\ S, \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{array} \right.$$

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

$$\chi^2(\mathbf{p}) = \chi_0^2 + (\mathbf{p} - \mathbf{p}_0)^T \mathbf{g}_0 + \frac{1}{2}(\mathbf{p} - \mathbf{p}_0)^T \mathbf{G}_0(\mathbf{p} - \mathbf{p}_0)$$

$$= \chi_0^2 + \Delta\chi^2.$$

$$\left\{ \begin{array}{l} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}} \chi^2(\mathbf{p}) \Big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}} \mathbf{g}(\mathbf{p}) \Big|_{\mathbf{p}=\mathbf{p}_0} \end{array} \right.$$

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

$$\text{cov}[\sigma_i(E)\sigma_j(E')] = \left[\nabla_{\mathbf{p}} \sigma_i(E) \right]^T \mathbf{C}_0 \left[\nabla_{\mathbf{p}} \sigma_j(E') \right] \Big|_{\mathbf{p}=\mathbf{p}_0}$$

$$= \Delta\sigma_i(E)\Delta\sigma_j(E')\rho_{ij}(E, E').$$

Parameter confidence intervals

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

$$\Delta\chi^2 = \frac{1}{2} \Delta\mathbf{p}^T \mathbf{G}_0 \Delta\mathbf{p} \leq \Delta\chi_{\max}^2,$$

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

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

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

$$\Delta p_i \leq \sqrt{2\Delta\chi_{\max}^2 H_{ii}} = \sqrt{\Delta\chi_{\max}^2 C_{ii}^0} \approx \sqrt{k C_{ii}^0},$$

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

Analyses

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□ ${}^7\text{Be}$

^7Be System Analysis

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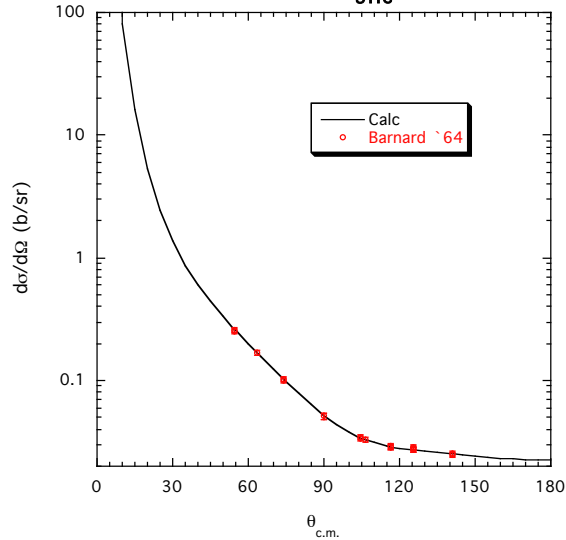
Channel	l_{\max}	a_c (fm)
$^3\text{He}+^4\text{He}$	4	4.4
$p+^6\text{Li}$	1	3.1
$\gamma+^7\text{Be}$	1	50

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

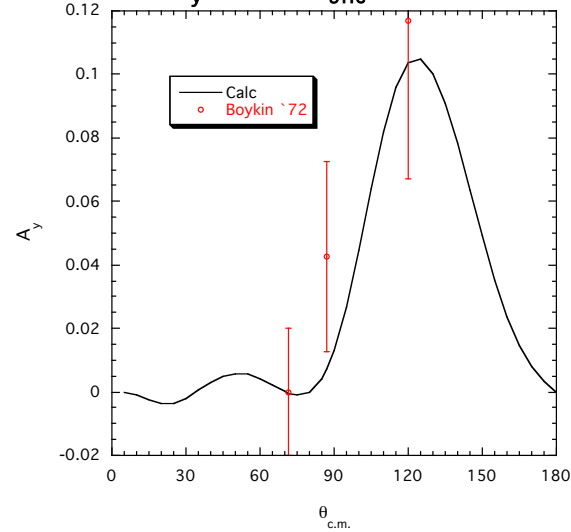
Example: $^3\text{He}+^4\text{He}$ Scattering

22

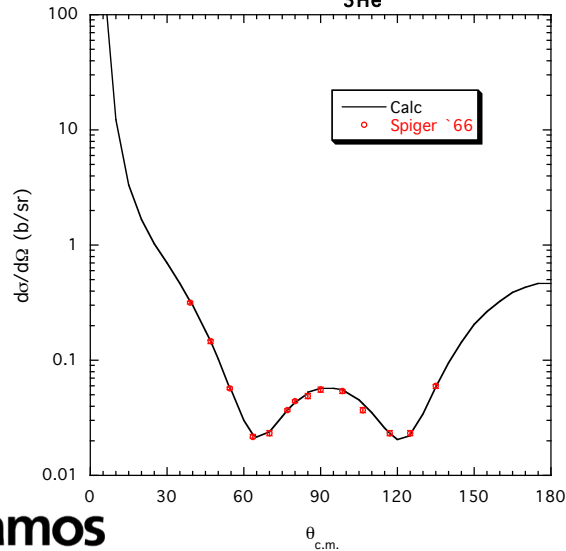
$^3\text{He}+^4\text{He}$ DXS @ $E_{^3\text{He}} = 3.6$ MeV



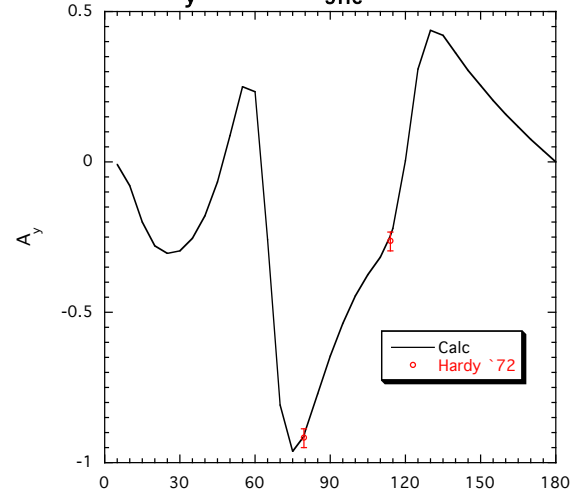
$A_y(^3\text{He})$ @ $E_{^3\text{He}} = 3.51$ MeV



$^3\text{He}+^4\text{He}$ DXS @ $E_{^3\text{He}} = 9.21$ MeV



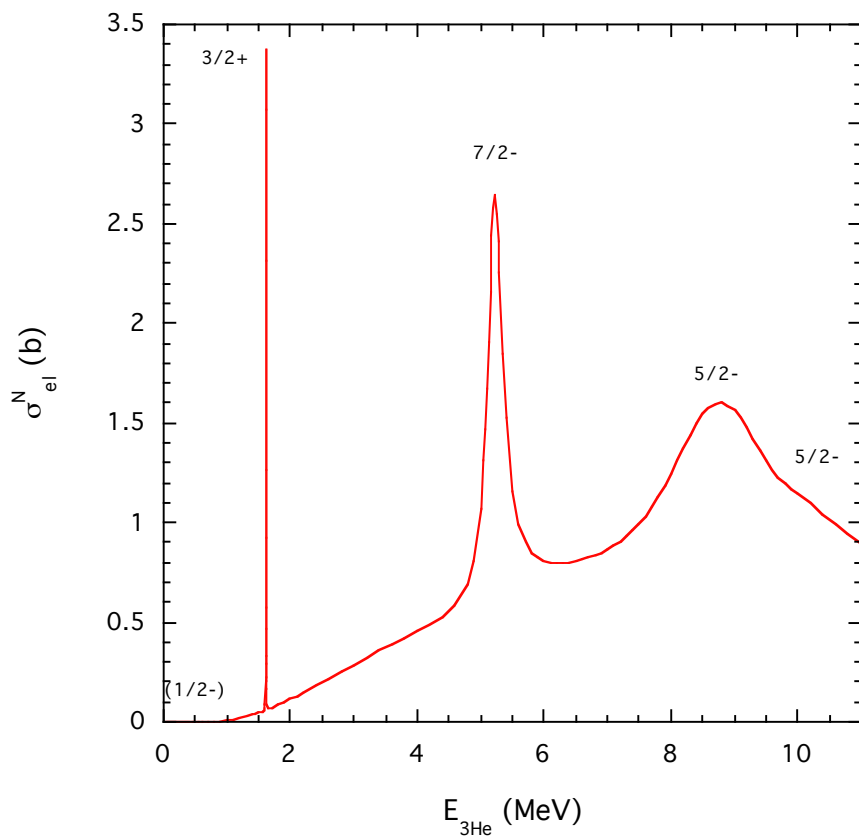
$A_y(^3\text{He})$ @ $E_{^3\text{He}} = 9.24$ MeV



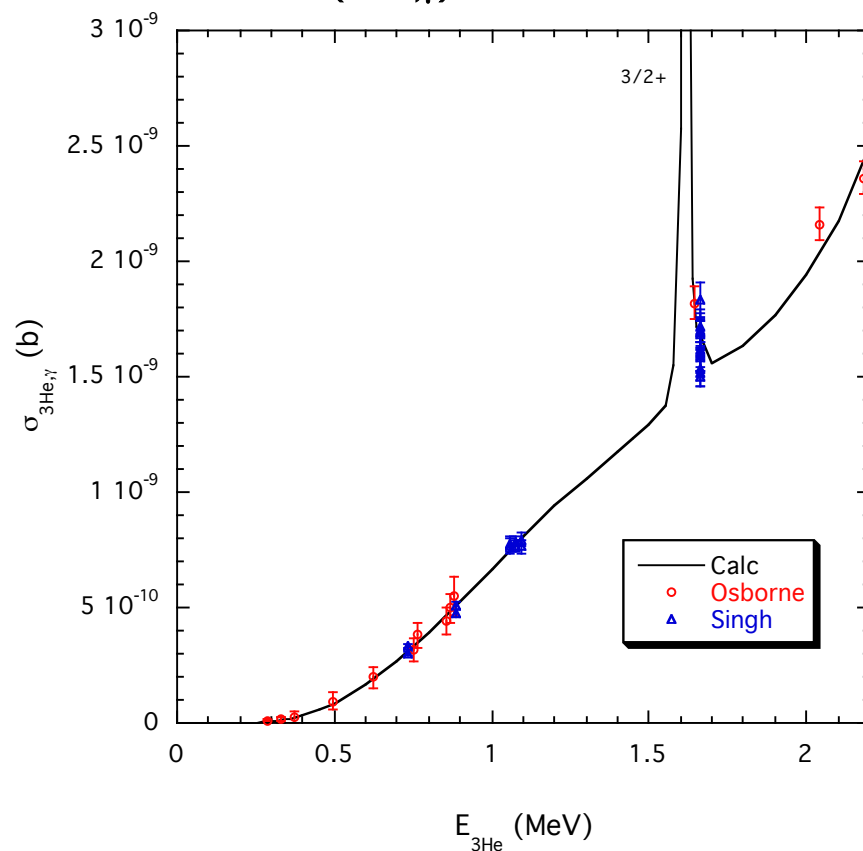
Resonances in the Cross Sections

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$^3\text{He} + ^4\text{He}$ Cross Section



$^4\text{He}(^3\text{He}, \gamma)^7\text{Be}$ Cross Section



^{17}O System Analysis

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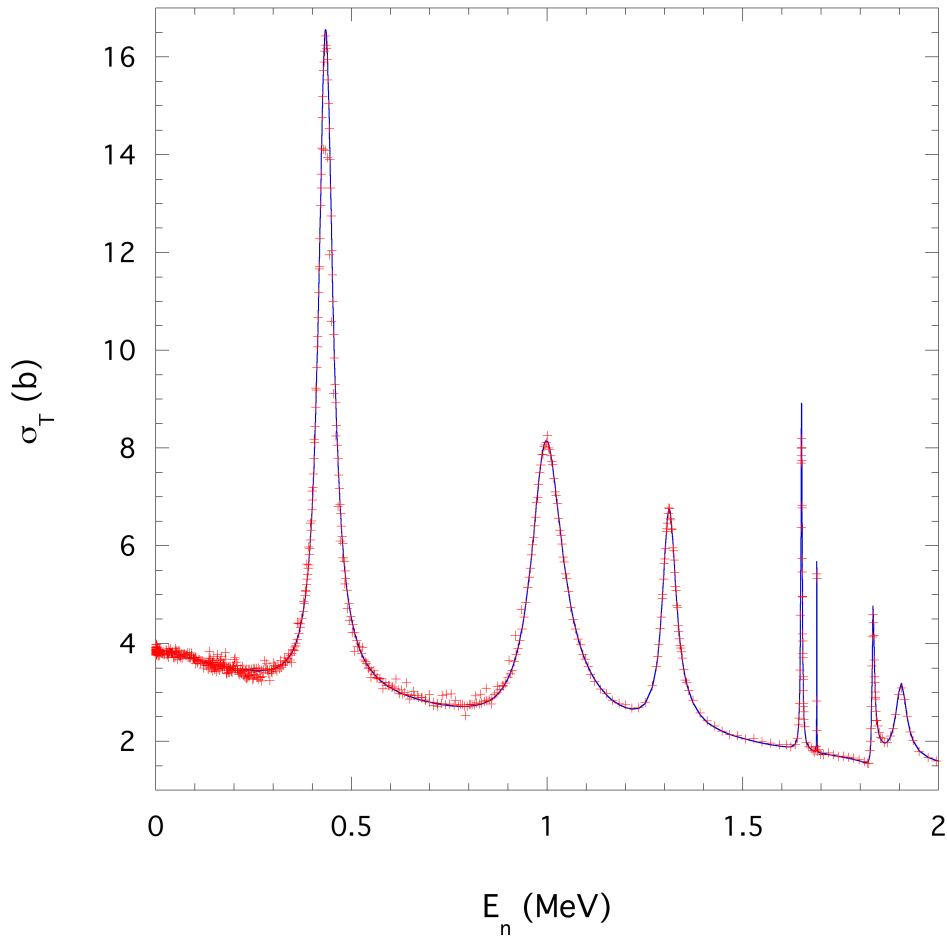
Channel	a_c (fm)	l_{\max}
$n+^{16}\text{O}$	4.3	4
$\alpha+^{13}\text{C}$	5.4	5

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

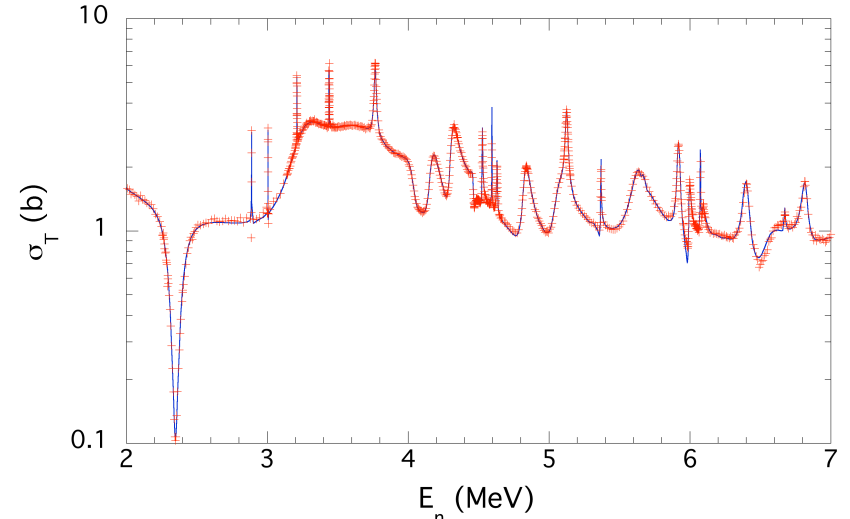
^{17}O System: comparison with data

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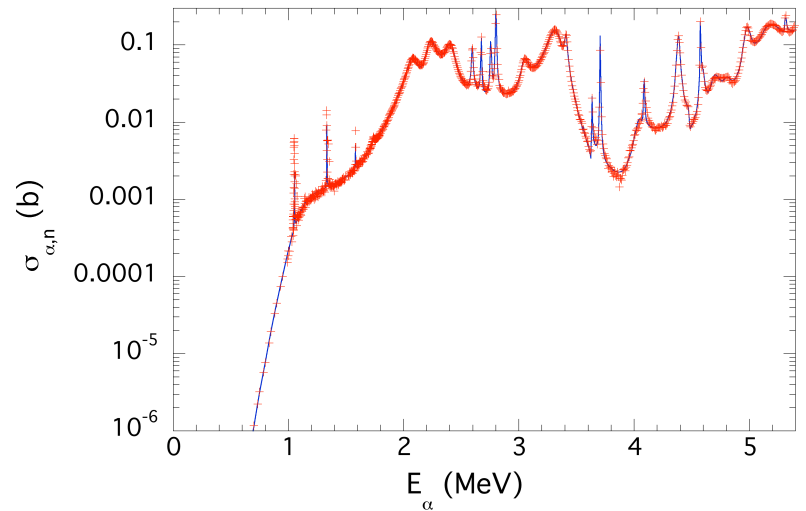
$n+^{16}\text{O}$ Total Cross Section



$n+^{16}\text{O}$ Total Cross Section



$^{13}\text{C}(\alpha,n)$ Cross Section

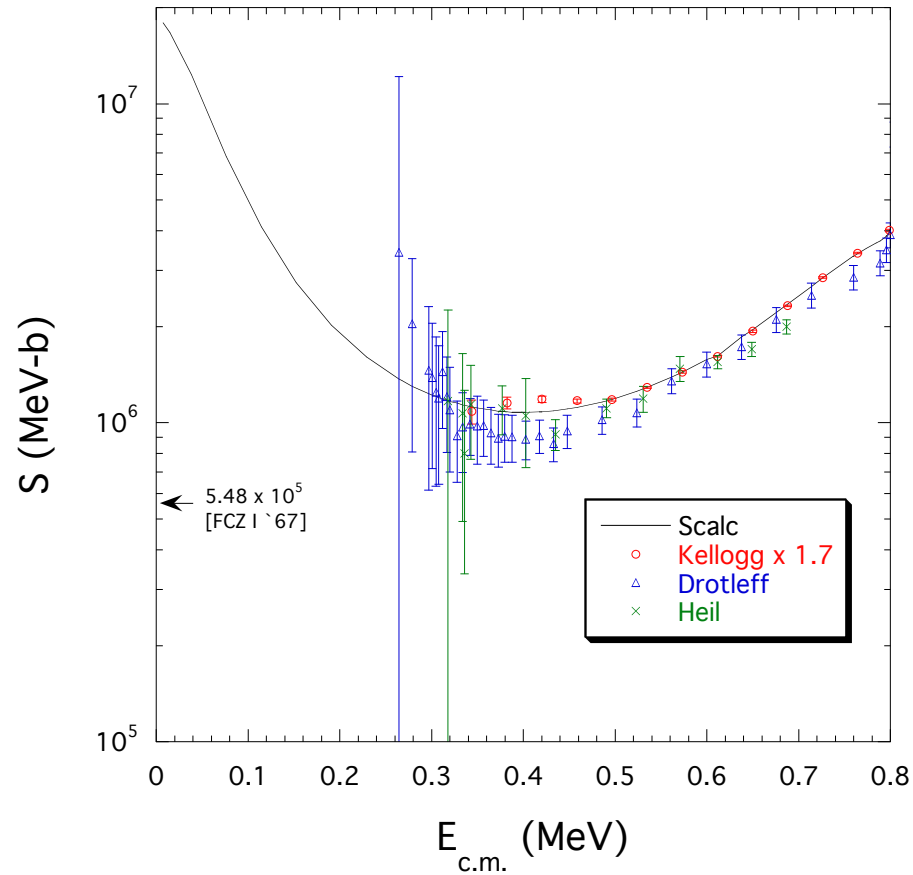


Paris & Hale (LANL)

R-Matrix Workshop 2016

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

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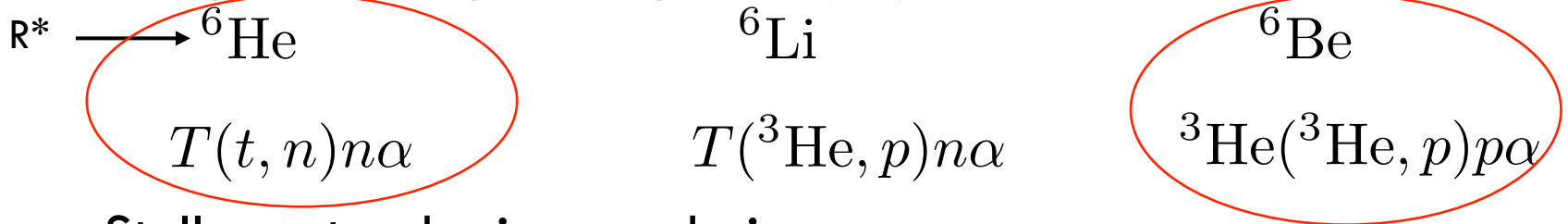


- 3-body final states are handled by the LANL auxiliary code SPECT

Motivation

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- Study $A=6$ compound systems (R^*)



- Stellar astrophysics: pp chain
- Cosmology: big bang nucleosynthesis ‘ ${}^7\text{Li}$ problem’
 - ▣ more neutrons from $T(t, n)n\alpha$ can destroy mass-7 via eg. ${}^7\text{Be}(n, p)$
- Inertial confinement fusion
 - ▣ OMEGA & NIF facilities are being used to study reactions of light nuclei

Collaborators

LANL: Hale, Herrmann, Kim, McEvoy,
Zylstra

OU: Brune

MIT: Frenje, Gatu-Johnson, Li, Petrasso

Rochester: Forrest, Knauer, Stoeckl

LLNL: Hohensee, McNabb, Pino, Sayre

Resonance model assumptions

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- Objective: use two-body data to describe three-body final states
- Approximate the three-body transition matrix as sum of sequential two-body decays

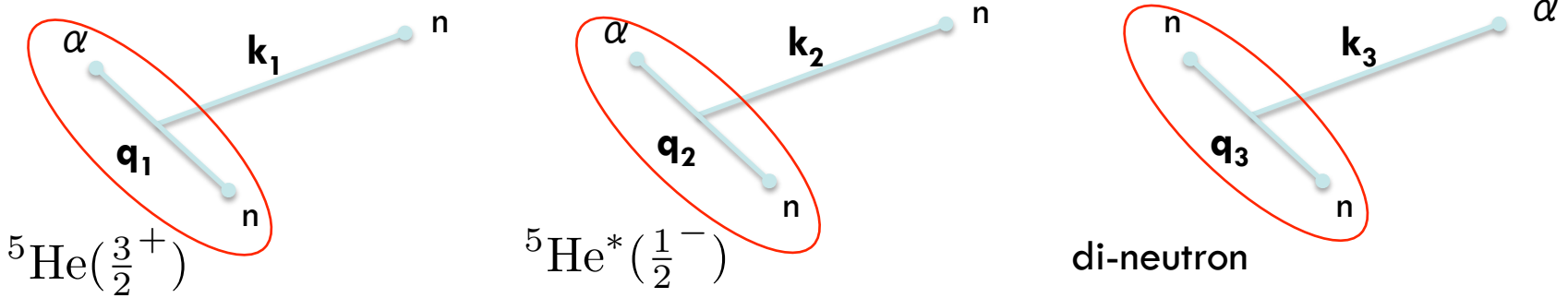
$$T^{(3)} = \sum_i^{N_c} c_i \tilde{T}_i^{(2)}$$

- Limit $N_c \rightarrow \infty$ this is exact; we approximate ∞ by 3(!): ‘Faddeev-like’
- Single level R-matrix description for $T_i^{(2)}$
- Interference between configurations ignored

Resonance model for 3-body final state (I)

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□ Configurations (T(t,n)n α)

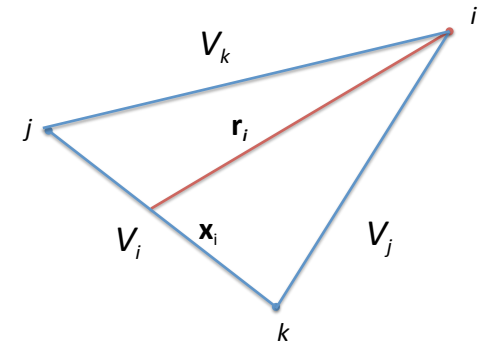


$$\frac{d^3\sigma}{d\mathbf{k}'_1} = \frac{(2\pi)^4}{v_{\text{rel}}} \int d^3k'_2 d^3k'_3 \left| T_{fi}^{(3)} \right|^2 \delta(\epsilon_i + Q - \epsilon_f)$$

$$T_{fi}^{(3)} = -\pi \langle \chi_f^{(3)} | \sum_i V_i | \psi_{\mathbf{k}_0}^{(+)} \rangle = -\pi \sum_i \langle \phi_{\mathbf{q}_i}^{(-)} \chi_{\mathbf{k}_i} | \hat{T}_i | \psi_{\mathbf{k}_0}^{(+)} \rangle$$

$$\phi^{(\pm)}(\mathbf{q}_i) = \chi_{\mathbf{q}_i} + G_{0,i}^{(\pm)}(\epsilon_{\mathbf{q}_i}) V_i \phi^{(\pm)}(\mathbf{q}_i)$$

$$\hat{T}_i = V_i + V_i G_{0,i}^+ V_i$$

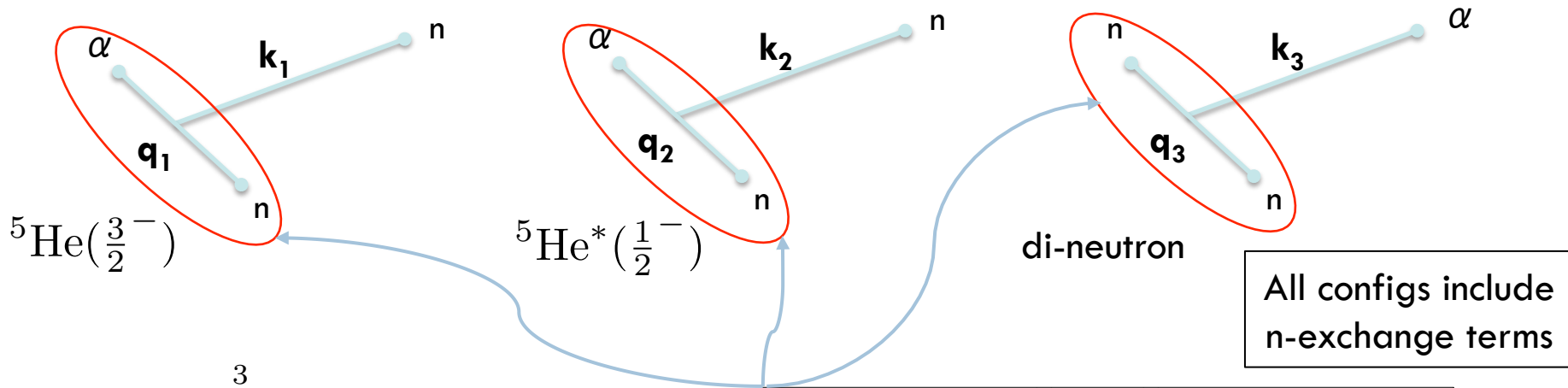


'Faddeev-like': two-body subsystems are not bound

Resonance model for 3-body final state (II)

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□ Configurations (T(t,n)nα)



All configs include n-exchange terms

$$T_{fi}^{(3)} = -\pi \sum_{i=1}^3 \langle \phi_{\mathbf{q}_i}^{(-)} \chi_{\mathbf{k}_i} | \hat{T}_i | \psi_{\mathbf{k}_0}^{(+)} \rangle$$

$$= \sum_{i=1}^3 \sum_{\lambda_i} c_{\lambda_i}^{(i)}(\mathbf{q}_i) \tilde{T}_{\lambda_i \mathbf{k}_i \mathbf{k}_0}^{(2)}$$

$$\tilde{T}_{\lambda \mathbf{k} \mathbf{k}_0}^{(2)} = \sum_{J s' \ell' s \ell} \mathcal{Y}_{J s' \ell'}(\hat{\mathbf{k}}) O_{\ell'}^{-1}(k)$$

$$\times R_{\lambda s' \ell' s \ell}^{\bar{L}}(\epsilon) O_{\ell'}^{-1}(k) \mathcal{Y}_{J s' \ell'}(\hat{\mathbf{k}}_0)$$

$$\phi_{\mathbf{q}}^{(-)} = \sum_{\lambda} c_{\lambda}^{(i)}(\mathbf{q}) \phi_{\lambda}^{(i)}(\mathbf{x})$$

$$\mathcal{L}_a |\phi^{(\pm)}\rangle = (H + \mathcal{L}_a - E) |\phi^{(\pm)}\rangle$$

$$c_{\lambda}^{(i)}(\mathbf{q}) = \frac{1}{\sqrt{\pi}} \sum_{\lambda'} A_{\lambda \lambda'} \gamma_{\lambda' i} O_i^{-1}(\mathbf{q}) \mathcal{Y}_i^{j \pi^*}(\hat{\mathbf{q}})$$

$$\sim \frac{1}{E_R - \frac{i}{2} \Gamma_R - \epsilon_q} e^{-i\phi_{\ell}} Y_{\ell}^0(\hat{\mathbf{q}})$$

Data fitting

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- Livermore '65 accelerator $T(t,n)n\alpha$
 - Recommended resolution broadening 0.5 MeV FWHM (determined from 14 MeV n peak)
 - Difficult to get realistic fit with 0.5 MeV at large E_n ; used 0.250 MeV & more narrow 'extended' R-matrix parameters
- OMEGA ${}^3\text{He}{}^3\text{He}$ data (courtesy A. Zylstra, LANL)
 - Scaled data (arbitrarily) to theory
 - should use total cross section
 - Gaussian thermal broadening 0.230 MeV
 - neglects small instrument broadening
- Least squares fit
 - parameters (next slide) $R_L^{(i)}$

Model parameters

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□ $T(t,n)n\alpha$

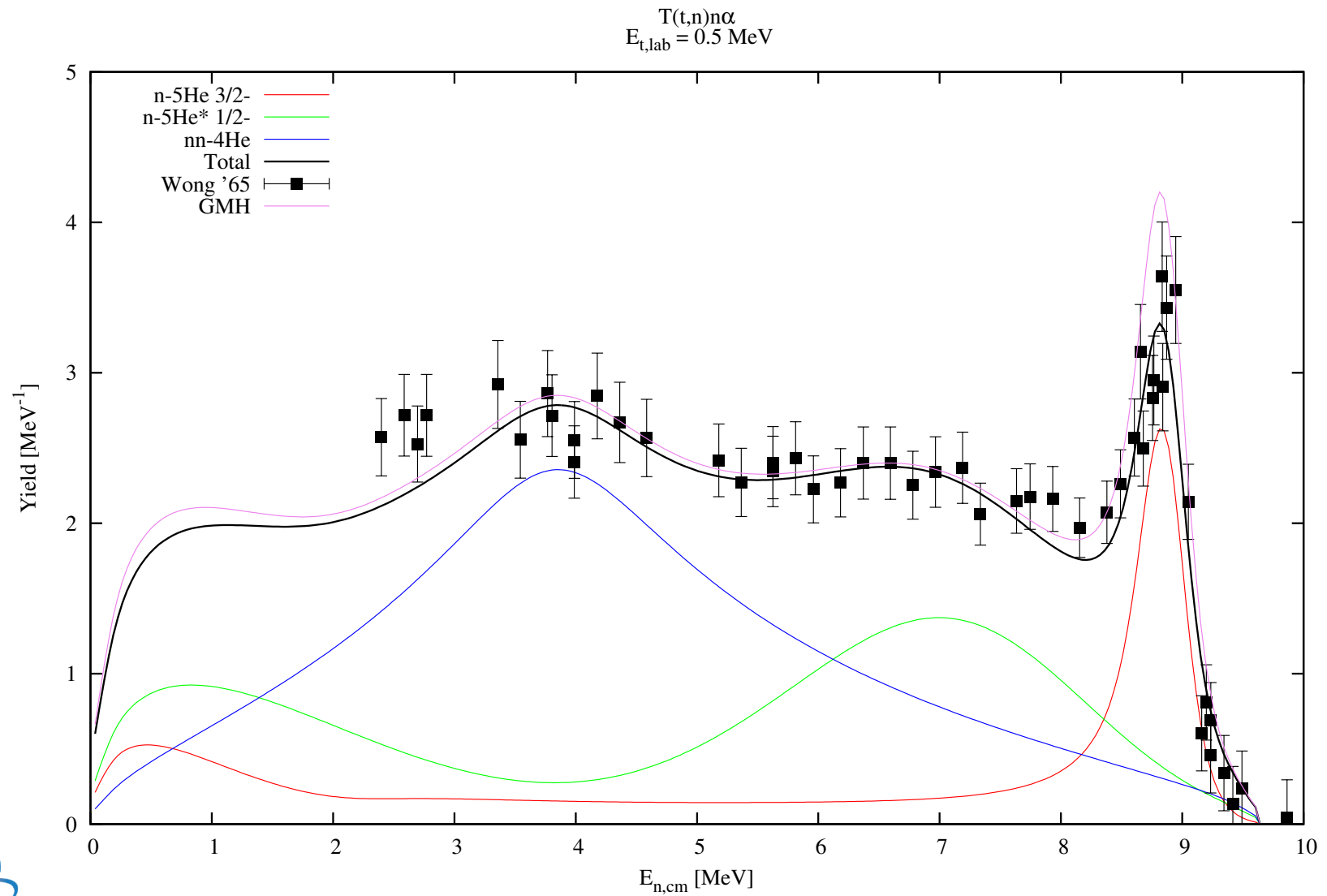
NPA 708 3 ('02)

Channel (resonance)	J^π	E_R (MeV)	Γ (MeV)	$ R^L $
$^5\text{He}+n$	$3/2^-$	0.99	0.65	0.157
$^5\text{He}^*+n$	$1/2^-$	6.66	20.6	0.547
$^4\text{He}+(nn)$	0^+	-0.07	0.	0.338

□ $^3\text{He}(^3\text{He},p)p\alpha$

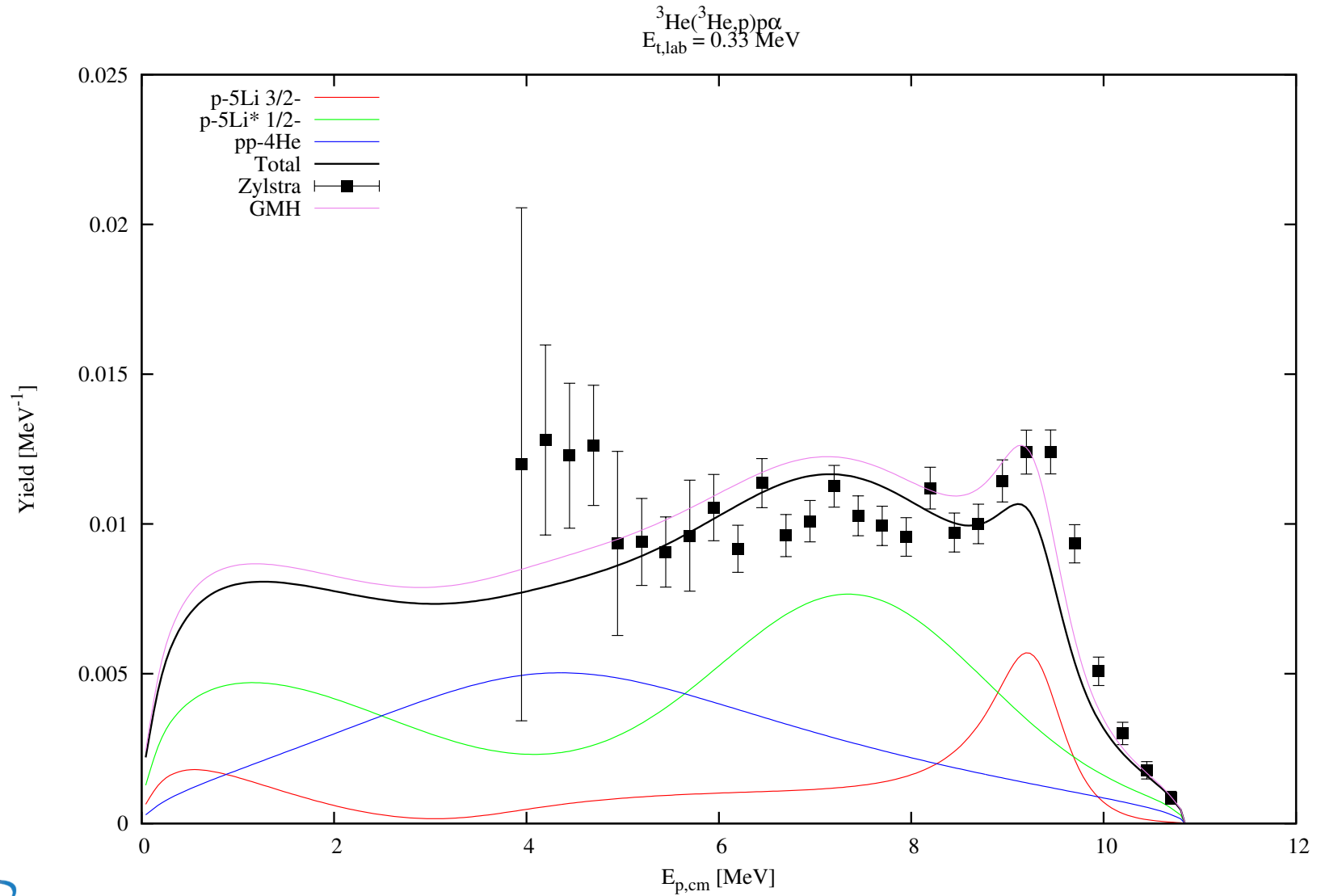
Fixed by 2-body data

Channel (resonance)	J^π	E_R (MeV)	Γ (MeV)	$ R^L $
$^5\text{Li}+p$	$3/2^-$	2.08	2.11	0.157
$^5\text{Li}^*+p$	$1/2^-$	8.26	19.8	0.547
$^4\text{He}+(pp)$	0^+	1.56	0.	0.234



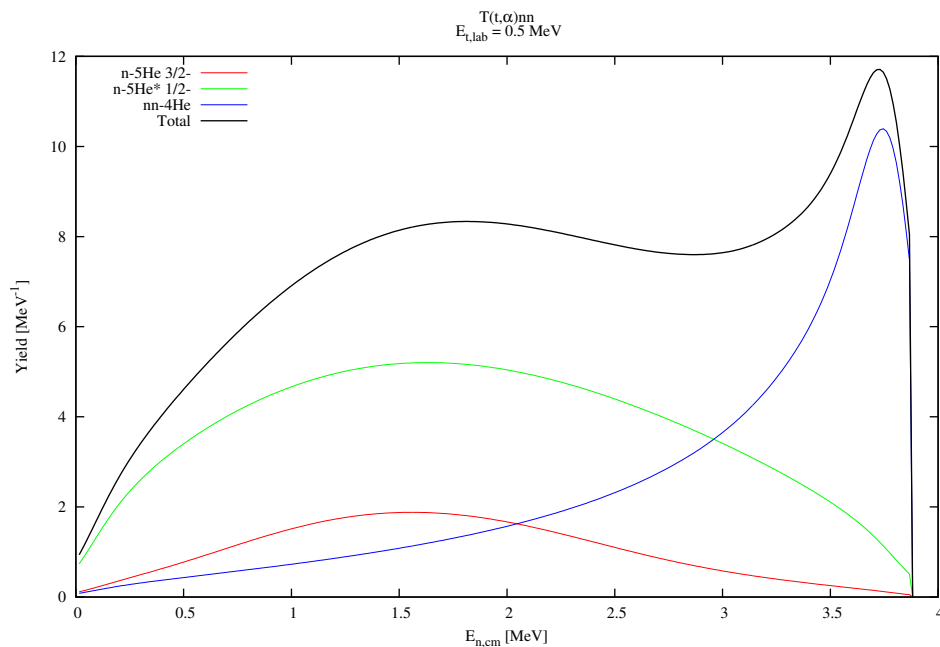
${}^3\text{He}({}^3\text{He}, p)p\alpha$

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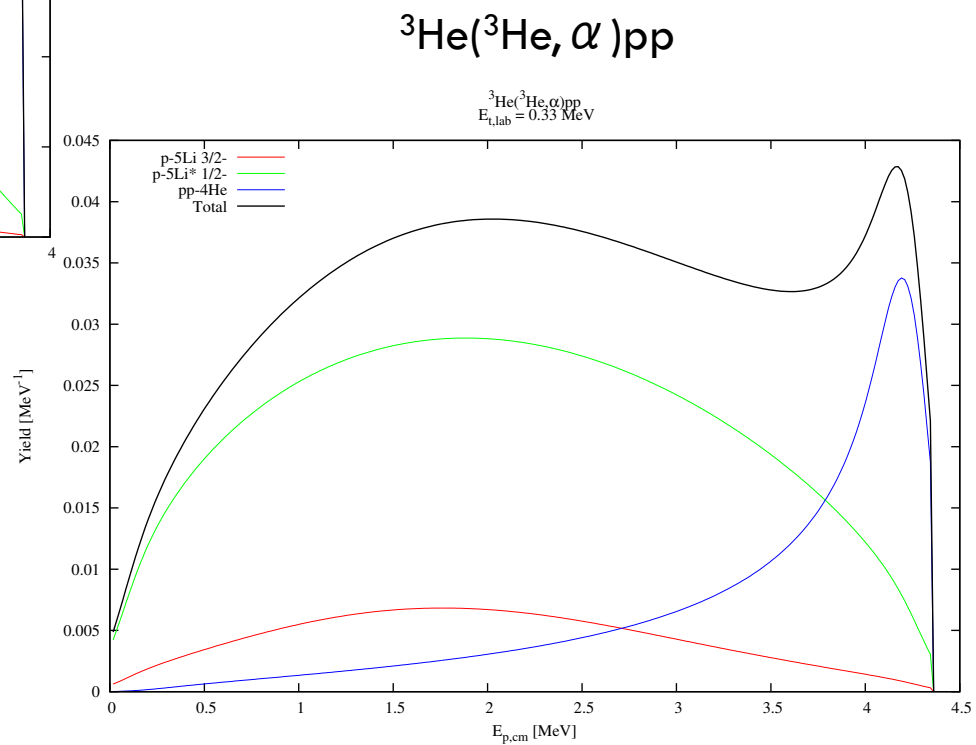


Alpha spectra

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$T(t, \alpha)nn$



Paris & Hale (LANL)

R-Matrix Workshop 2016

Planned improvements

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- Data
 - Incorporate all OMEGA $^3\text{He}^3\text{He}$ & ^3HeT
 - Include NIF TT
 - α spectra
- Fitting
 - Non-linear least squares
 - Marquardt-Levenberg; gradient; etc.
- Model
 - Angular dependence nn wave function
 - Incident energy dependence

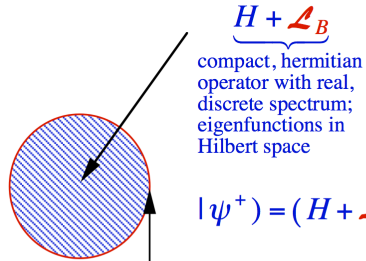
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Follow-on material

2→2 body R matrix formalism

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INTERIOR (Many-Body) REGION
(Microscopic Calculations)



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

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

or equivalently,

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

Measurements

SURFACE

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

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

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

□ Channels: $r_c = a_c$

□ not nec. nucl. surface; regulator

$$\square \exists F : R_B(a_c) \xrightarrow{F} R_{B'}(a'_c)$$

$$\text{and } T \xrightarrow{F} T$$

□ Sturm-Liouville eigenvalue prob.

□ BC at finite a_c

□ complete set $|\lambda\rangle$

□ Hermiticity: $(H + \mathcal{L}_B)^\dagger = H + \mathcal{L}_B$

□ Bloch operator

$$\mathcal{L}_{BC} \psi_c^{(+)} = 0 \Leftrightarrow \frac{1}{r_c \psi_c^{(+)}} \frac{\partial}{\partial r_c} r_c \psi_c^{(+)} \Big|_{a_c} = B_c$$

□ T matrix

$$T = O^{-1} R_L O^{-1} - O^{-1} F$$

$$B_c = L_c = \frac{r_c}{O_c} \frac{\partial O_c}{\partial r_c} \Big|_{r_c = a_c}$$

$$R_B^{-1} + B = R_{B'}^{-1} + B'$$

Analyses

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□ ^5He

R-matrix analysis of ^5He system

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^5He Analysis

Channel	l_{max}	a_c (fm)
d-t	5	5.1
n- ^4He	5	3.0
n- $^4\text{He}^*$	1	5.0
γ - ^5He	1	60.

Reaction	Energy Range	# Obs. Types	# Data Points	χ^2
T(d,d)T	$E_d=0-8.6$ MeV	6	700	1231
T(d,n) ^4He	$E_d=0-11$ MeV	14	1185	1523
T(d,n) $^4\text{He}^*$	$E_d=4.8-8.3$ MeV	1	10	18
T(d, γ) ^5He	$E_d=0-8.6$ MeV	2	17	29
$^4\text{He}(n,n)^4\text{He}$	$E_n=0-28$ MeV	2	817	1117

Totals 25 2729 3918

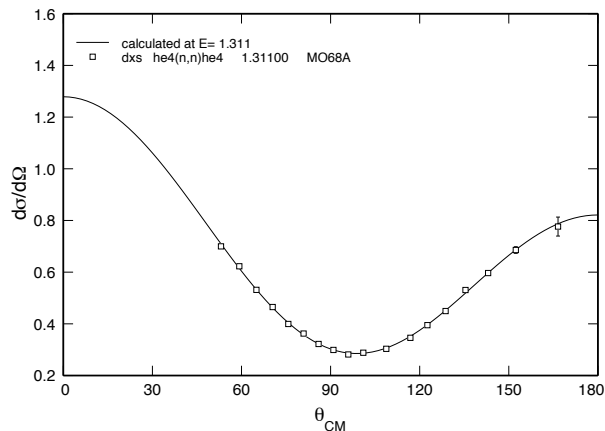
parameters = 117 $\Rightarrow \chi^2$ per degree of freedom = 1.50

[109 phase parameters are necessary to describe the S matrix at a single energy]

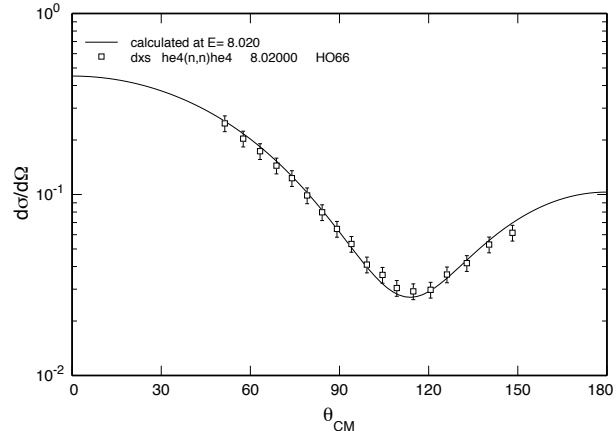
$^4\text{He}(n,n)^4\text{He}$ differential cross section

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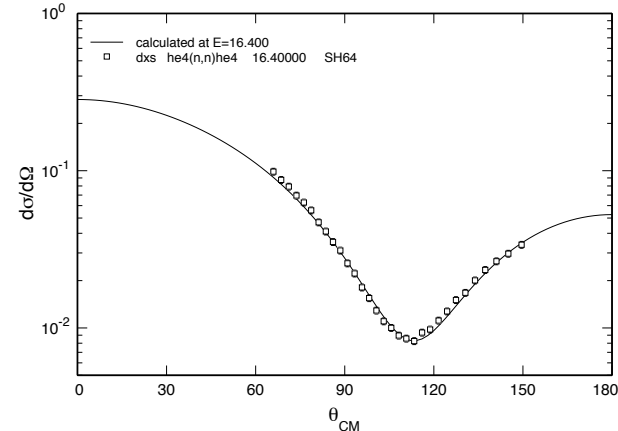
he4(n,n)he4 $d\sigma/d\Omega$ E= 1.311 MeV



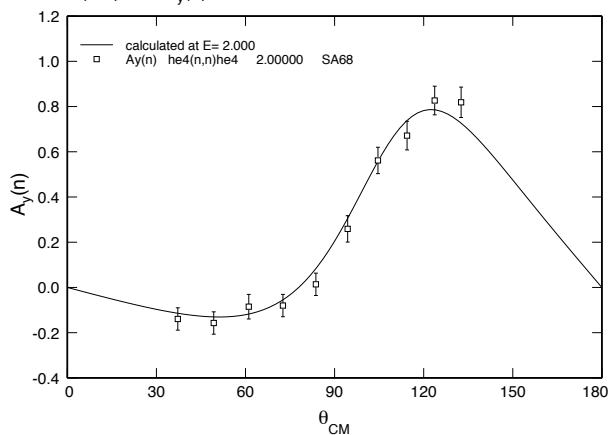
he4(n,n)he4 $d\sigma/d\Omega$ E= 8.020 MeV



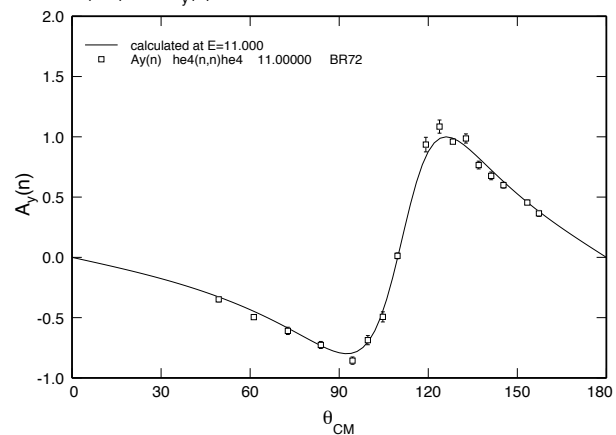
he4(n,n)he4 $d\sigma/d\Omega$ E=16.400 MeV



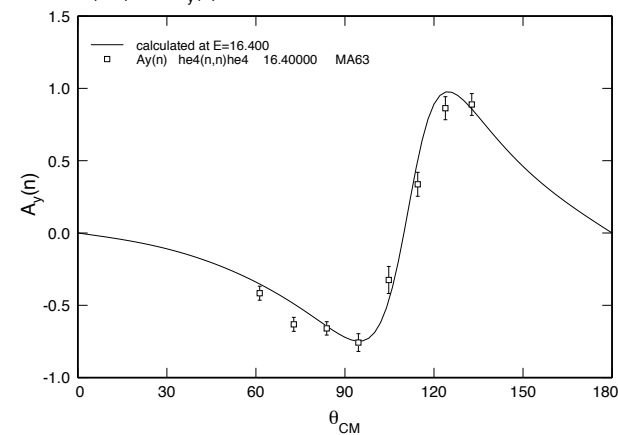
he4(n,n)he4 $A_y(n)$ E= 2.000 MeV



he4(n,n)he4 $A_y(n)$ E=11.000 MeV



he4(n,n)he4 $A_y(n)$ E=16.400 MeV



Integrated cross section

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