70 YEARS OF CREATING TOMORROW

Los Alamos NATIONAL LABORATORY

Reflections on the History of R-Matrix Theory and its Application to Light Nuclear Reactions

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Outline

- Brief survey of important papers
- Introduction to Green's function, Bloch operator *R*-matrix theory
- *R* matrices for different choices of boundary condition
- Kapur-Peierls *R* matrix, *T*-matrix poles and resonance parameters
- Humblet-Rosenfeld objections to *R*-matrix theory
- Approximate chronology of *R*-matrix codes
- Example: EDA analysis of reactions in ^{5}He system
- A brief encounter with Wigner
- Unphysical extension of the theory to zero channel radius; connection with EFT (ex: n-p scattering)
- Summary of the past, new directions for the future

Landmark and Other Significant Papers

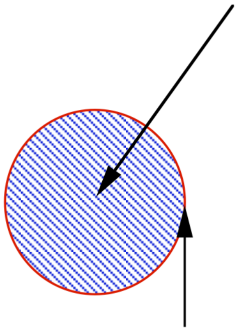
Year	Author(s)	Journal Ref.	Comment
1938	Kapur and Peierls	Proc. Roy. Soc. A **166,** 277-295	2-region, n.p. approach to derive dispersion formula
1947	Wigner and Eisenbud	Phys. Rev. **72**, 29-41	Beginning of standard R-matrix theory
1957	Claude Bloch	Nucl. Phys. **4**, 503-528	Bloch operator, distant levels ⇔ direct reactions
1958	Lane and Thomas	Rev. Mod. Phys. **30**, 257-353	The "bible"
1966	Lane and Robson	Phys. Rev. **151**, 774-787	Modern approach using the Bloch operator
2002	Carl Brune	Phys. Rev. C **66**, 044611, 1-8	Alternative parametrization (R_S)
2010	Descouvemont and Baye	Rep. Prog. Phys. **73**, 036301, 1-44	Calculable R matrix

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.)

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

or equivalently,

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

Measurements

R Matrices for General Boundary Conditions in the Bloch Operator

$$B_c \rightarrow X_c(E)$$

$$\begin{aligned}\mathbf{R_X} &= (c' \,|\, (H + \mathcal{L}_X - E)^{-1} \,|\, c) \\ &= (\Lambda - \mathbf{X})^{-1} \\ &= [\mathbf{1} - \mathbf{R_B}(\mathbf{X} - \mathbf{B})]^{-1}\mathbf{R_B}\end{aligned}$$

Most common choices are **X** = **L** = **S** + *i* **P**, and **X** = **S**.

The real poles and residues of $\mathbf{R_S}$ are often used to give resonance parameters, and that is the basis of Carl Brune's alternative *R*-matrix parametrization. However, the real-energy resonance pole prescription is fundamentally different from the complex-momentum one, and gives different results even in the simplest cases.

The Kapur-Peierls R-matrix, R_L

$$\mathbf{R_L} = (c' | \underbrace{(H + \mathcal{L}_L - E)^{-1}}_{G_L = -G^+(E)} | c)$$

$$= (\Lambda - \mathbf{L})^{-1}$$

$$= [\mathbf{1} - \mathbf{R_B}(\mathbf{L} - \mathbf{B})]^{-1}\mathbf{R_B}$$

$$= [\mathbf{1} - i\mathbf{R_S}\mathbf{P}]^{-1}\mathbf{R_S}$$

Solving the fundamental R-matrix relation, $\psi^+ = (H + \mathcal{L}_L - E)^{-1}\mathcal{L}_L\psi^+$, for the transition matrix gives

$$\mathbf{T} = \mathbf{O}^{-1}\mathbf{R_L}\mathbf{O}^{-1} \quad \underbrace{-\mathbf{FO}^{-1}}_{\text{hard-sphere amplitude}} \quad \left\{ O_c^{-1} = P_c^{\frac{1}{2}} \exp(-i\phi_c) \text{ at real energies} \right.$$

- Most directly related to the asymptotic scattering amplitudes
- Poles of $\mathbf{R_L}$ are the poles of **T** (or **S** = **1** + 2*i* **T**).
- Awkward to parameterize directly; more easily expressed in terms of $\mathbf{R_B}$ or $\mathbf{R_S}$

R_B and R_L

W/E boundary conditions:

B_c real, energy-independent.

$$R^B_{c'c} = \sum_\lambda \frac{\gamma_{c'\lambda}\gamma^{\mathrm{T}}_{\lambda c}}{E_\lambda - E}$$

is real, symmetric, TRI, unitary.

K/P boundary conditions:

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

complex, energy-dependent.

$$R^L_{c'c} = \sum_{\lambda'\lambda} \gamma_{c'\lambda'} A_{\lambda'\lambda}(E)\gamma^{\mathrm{T}}_{\lambda c}$$

$$A^{-1}_{\lambda'\lambda}(E) = (\lambda' | H + \mathcal{L}_L - E | \lambda)$$

$$= (E_\lambda - E)\delta_{\lambda'\lambda} - \gamma^{\mathrm{T}}_{\lambda' c}(L_c - B_c)\gamma_{c\lambda}$$

$\mathbf{R_L} = [\mathbf{1} - \mathbf{R_B}(\mathbf{L} - \mathbf{B})]^{-1}\mathbf{R_B}$ is the outgoing-wave Green's function projected onto the channel surface; its poles are those of the *T*-matrix, given by

$$\mathbf{T} = \mathbf{O}^{-1}\mathbf{R_L}\mathbf{O}^{-1} \underbrace{-\mathbf{F}\mathbf{O}^{-1}}_{\text{hard-sphere amplitude}} \quad \left\{ O_c^{-1} = P_c^{\frac{1}{2}} \exp(-i\phi_c) \text{ at real energies} \right.$$

Approach: use $\mathbf{R_B}$ for fitting experimental data and $\mathbf{R_L}$ for interpreting results

Properties of R_B and R_L

R_B is a meromorphic function with poles only on the real energy axis.

The analytic structure of R_L is more complicated, with poles (in k) in the complex plane, and cuts along the real energy axis.

The eigenfunctions of $H+\mathcal{L}_B$ form a complete, orthogonal set in the internal region. The eigenenergies of the expansion are real.

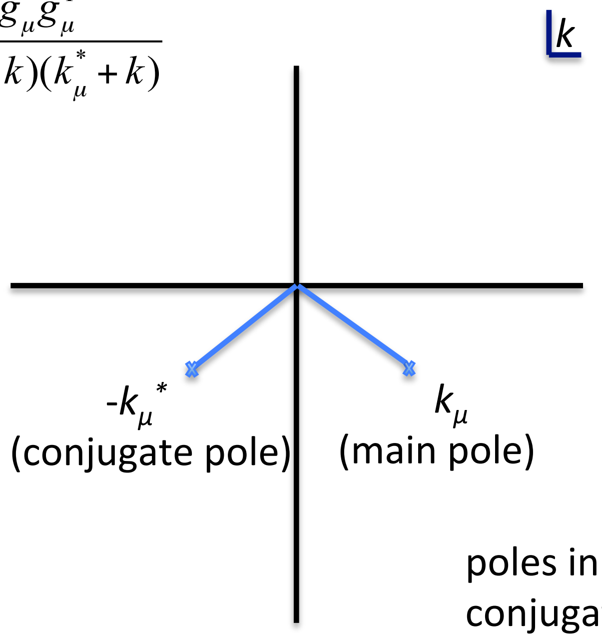
The eigenfunctions of $H+\mathcal{L}_{L(E)}$ for fixed energy form a complete, bi-orthogonal set in the internal region. The eigenenergies of the expansion are complex. This was the original idea of the Kapur-Peierls expansion, but its parameters are energy-dependent and complex. Using the "true" poles of R_L gets rid of the energy dependence, but the associated eigenfunctions are no longer complete or bi-orthogonal (part of a Berggren basis).

Therefore, R_B has the nicest mathematical properties, but is the hardest to interpret. R_L expansions are much messier, but its poles and residues are directly connected to resonances.

Scattering Properties Ensured by R_L

- Unitarity follows from Im $\mathbf{R_L} = \mathbf{R_L P R_L^*}$
- Causality and Reciprocity follow from the pole structure of R_L in the complex k-plane:

$$R_L = \frac{2\mu}{\hbar^2}\frac{g_\mu g_\mu^{\mathrm{T}}}{(k_\mu - k)(k_\mu^* + k)}$$



poles in lower half-plane ⇒ causality
conjugate pole (symmetry about imaginary axis) ⇒ TRI

Resonance Parameters (RP) Derived from R_L

Near a pole of T at $E = E_\mu$ $(k = k_\mu)$ on an unphysical sheet,

$$\mathbf{T} \approx \mathbf{O}^{-1} \frac{\mathbf{g}_\mu \mathbf{g}_\mu^{\mathrm{T}}}{E_\mu - E} \mathbf{O}^{-1} = \frac{1}{2} \frac{\boldsymbol{\Gamma}_\mu^{\frac{1}{2}} \boldsymbol{\Gamma}_\mu^{\frac{1}{2}\,\mathrm{T}}}{E_\mu - E} \quad \begin{cases} \Gamma_{c\mu} = 2\left|g_{c\mu}\right|^2 \left|O_c(k_\mu)\right|^{-2}, \\ E_\mu = \dfrac{\hbar^2}{2\mu} k_\mu^2 = E_r - \dfrac{1}{2} i \Gamma_\mu \end{cases}$$

However, $\Gamma_\mu = -2\Im E_\mu = 2\sum_c \left|g_{c\mu}\right|^2 \Im L_c(k_\mu) \neq \sum_c \Gamma_{c\mu}$ unless $\Im L_c(k_\mu) = \left|O_c(k_\mu)\right|^{-2}$.

This is true on the real axis, but not in the complex plane. Therefore, define the "strength" of a resonance by

$$s = \frac{\sum_c \Gamma_{c\mu}}{\Gamma_\mu} \approx 1 \text{ for a narrow resonance.}$$

Humblet-Rosenfeld Objections to R-Matrix Theory

- Boundary conditions B_c are arbitrary.
  - True, but they can be chosen to have physical significance, as e.g., "natural" b.c. $B_c = S_c(\bar{E})$, or $S_c(0) \approx -l_c$.
  - Fred Barker showed how to transform *R*-matrix parameters analytically from one fixed boundary condition to another.
- Channel radii a_c seem arbitrary.
  - On the contrary, they give useful information about the sizes of the interacting particles and the range of nuclear forces.
  - Poles and residues of asymptotic amplitudes (such as *T*) are formally independent of a_c since the boundary conditions are logarithmic derivatives of solutions of the Schrödinger Eqn.
- On the basis of these objections, H&R developed a (flawed) *K*-matrix expansion for nuclear reactions, and Rosenfeld, a Senior Editor for *Nuclear Physics*, refused to consider any *R*-matrix submissions to the journal for more than a decade.

Radial Independence of RPs Derived from R_L

At the resonance energy, $W(\mathbf{O},\mathbf{U})\big|_{r_c=a_c,E=E_\mu} = \mathbf{O}\mathbf{U}' - \mathbf{O}'\mathbf{U} = 0$, expressing the condition that the radial solution matrix **U** is proportional to the outgoing-wave solutions at the channel surface. This Wronskian condition also holds for all radii $r_c > a_c$, establishing the radial independence of the resonance energy E_μ.

Similarly, the fact that $g_{c\mu} \propto O_c(k_\mu)$ means that $\Gamma_{c\mu} = 2|g_{c\mu}|^2 |O_c(k_\mu)|^{-2}$ is also formally independent of channel radius for $r_c > a_c$. Thus, both the partial widths $\Gamma_{c\mu}$ and the total width $\Gamma_\mu = -2\Im E_\mu$ are independent of channel radius, meaning that the strength is also.

The radial independence of these parameters has been observed in practice for the two lowest-lying resonances in ^{5}He ($3/2^-$, $1/2^-$), using the *n*-α *R*-matrix parameters of Barker that were defined at a much larger radius than we used in our ^{5}He analysis.

(Note that this formal radial independence does not apply for real-energy resonance parameters derived from $\mathbf{R_S}$.)

Nuclear R-matrix Analysis Codes

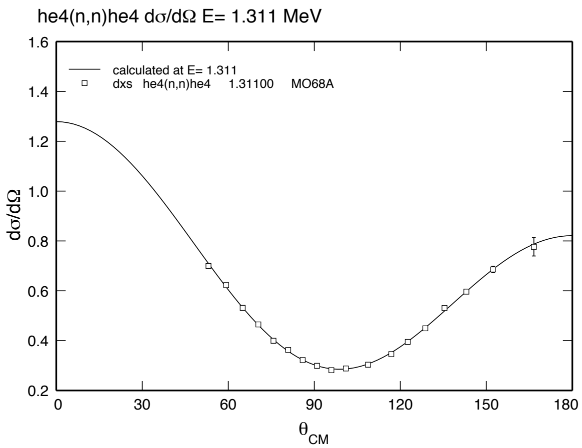
~ Year	Code Name	particles	kinematics	observables
1968	MULTI	n,c	n.r.	σ(E), σ(θ)
1972	EDA	n,c,γ	rel. (and n.r.)	all
1974	MULTI	n	n.r.	σ(E)
1978	ORMAP	n,c	n.r.	σ(E), σ(θ) , P(θ)
1978	RFUNC	n	n.r.	σ(E)
1980	SAMMY	n,c,γ	n.r.	σ(E), σ(θ)
1990	RAC	n,c,γ	n.r.	σ(E), σ(θ), P(θ)
2005	CONRAD	n,c	n.r.	σ(E), σ(θ)
2006	SFRESCO	n,c,γ	rel. (and n.r.)	all
2009	REFIT	n	n.r.	σ(E)
2010	AZURE	n,c,γ	n.r.	σ(E), σ(θ)
2012	AMUR	n,c,γ	n.r.	σ(E), σ(θ)
2013?	HYRMA	n,c	n.r.	σ(E), σ(θ)

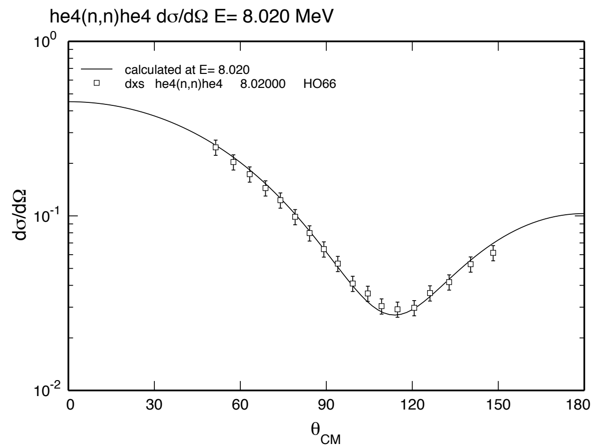
Analysis of Reactions in the ^{5}He System

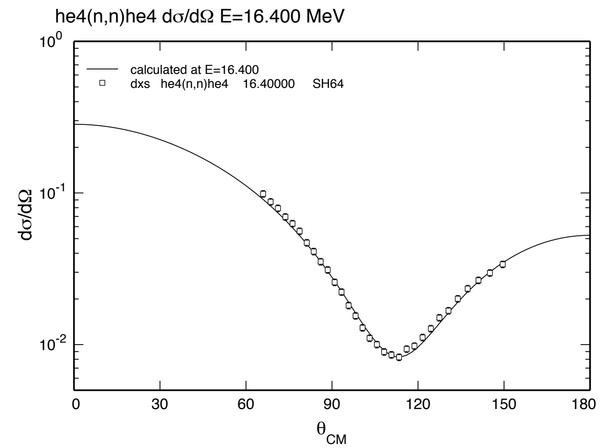
channel	a_c (fm)	l_{max}
n+^{4}He	3.0	5
γ+^{5}He	60	1
d+^{3}H	5.1	5
n+^{4}He*	5.0	1

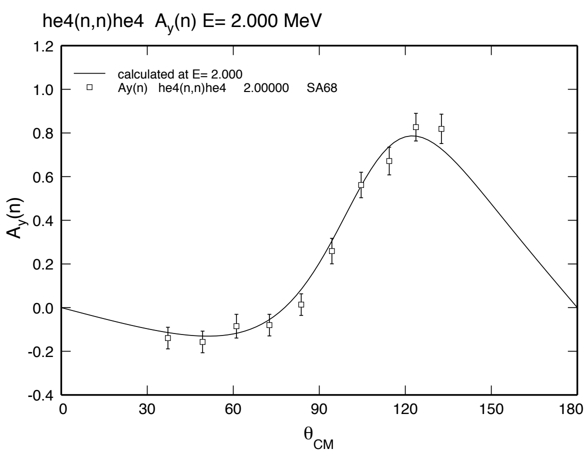
Reaction	Energies (MeV)	# data points	# data types
^{4}He(n,n)^{4}He	E_n = 0 – 28	817	2
^{3}H(d,d)^{3}H	E_d = 0 – 8.6	700	6
^{3}H(d,n)^{4}He	E_d = 0 – 11	1185	14
^{3}H(d,γ)^{5}He	E_d = 0 – 8.6	17	2
^{3}H(d,n)^{4}He*	E_d = 4.8 – 8.3	10	1
total		2729	25

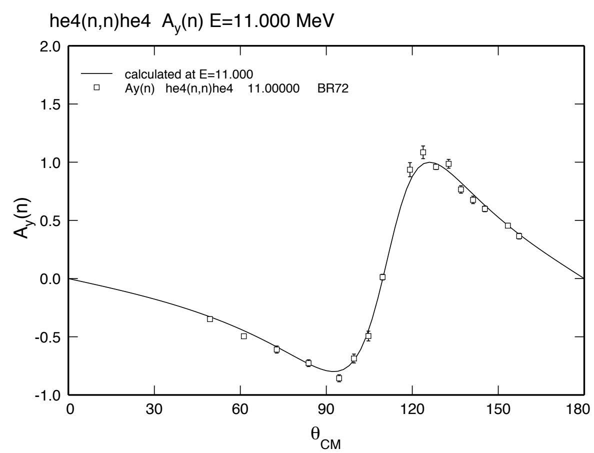
$^{4}He(n,n)^{4}He$ Scattering

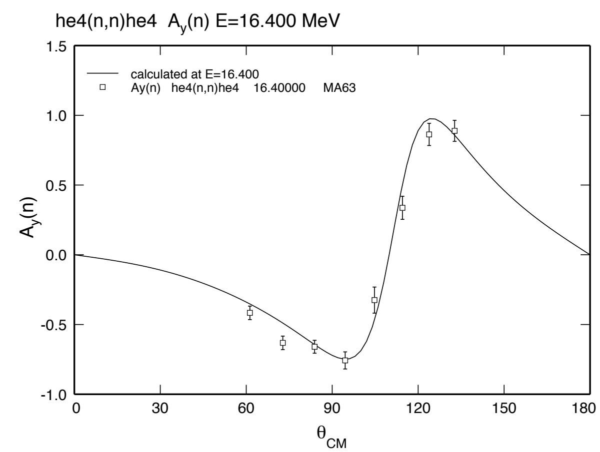




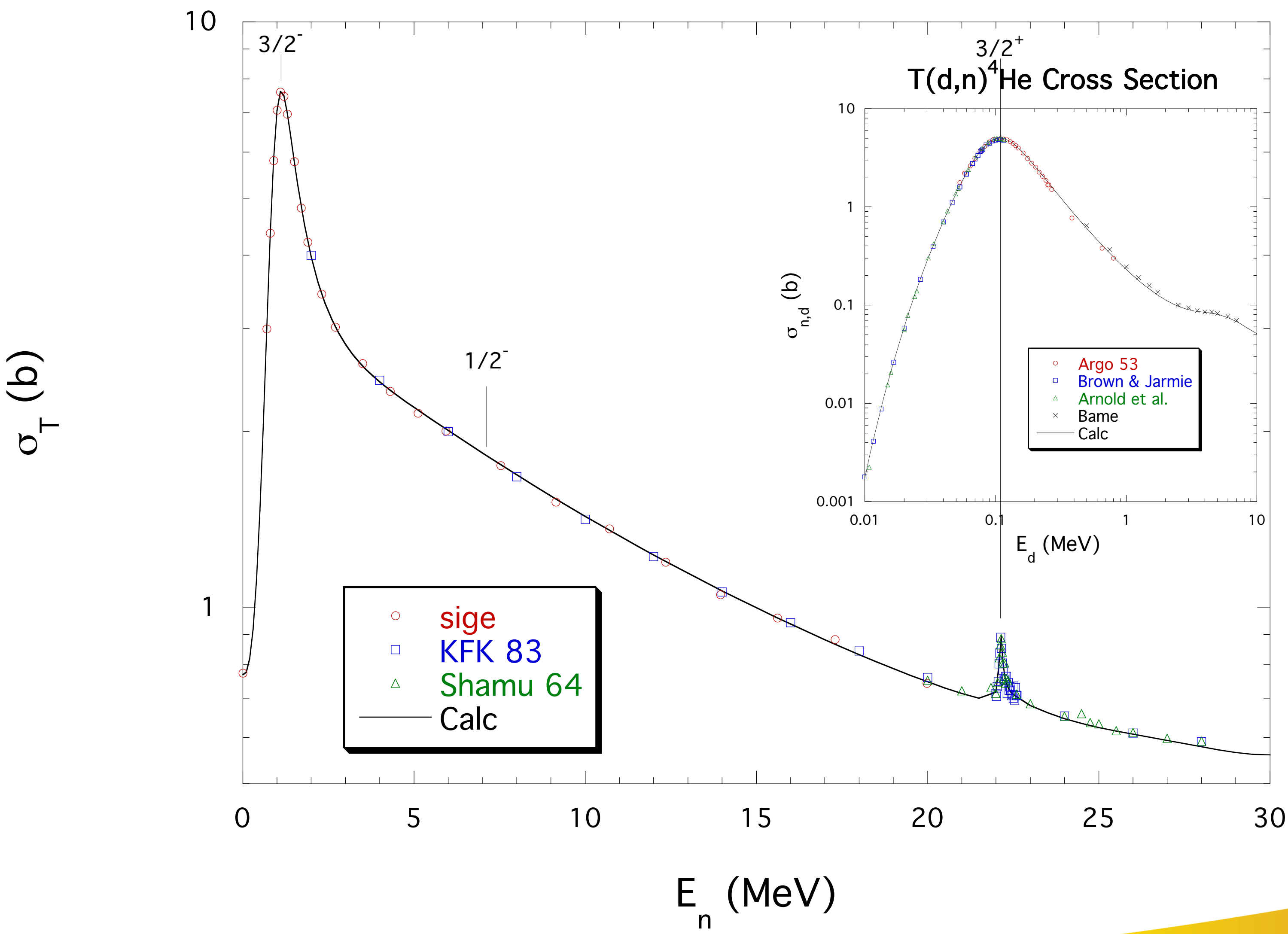




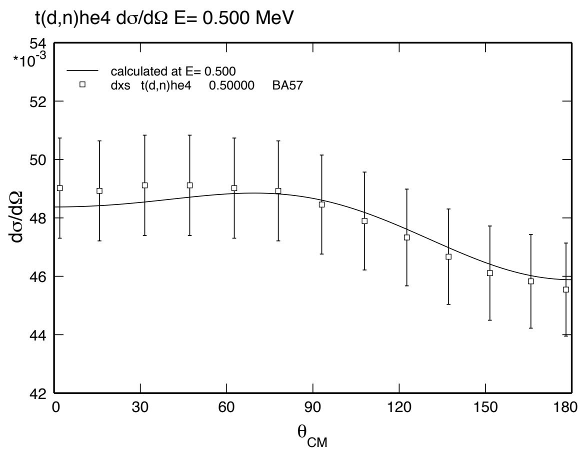


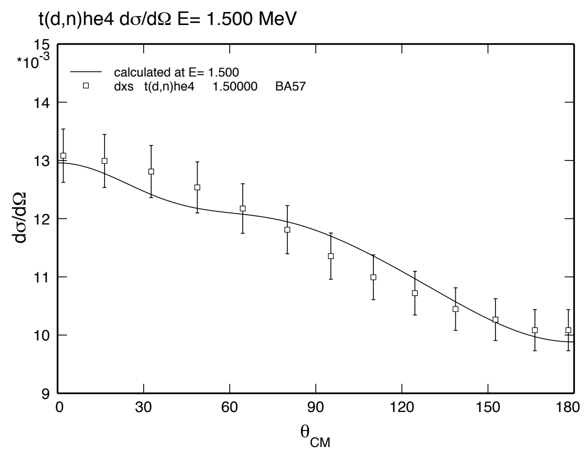


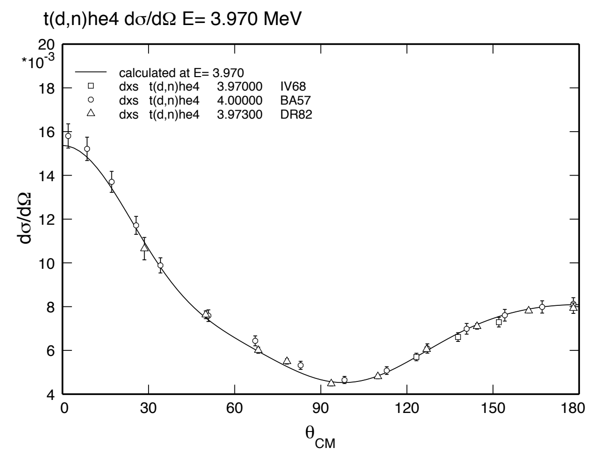
Integrated Cross Sections

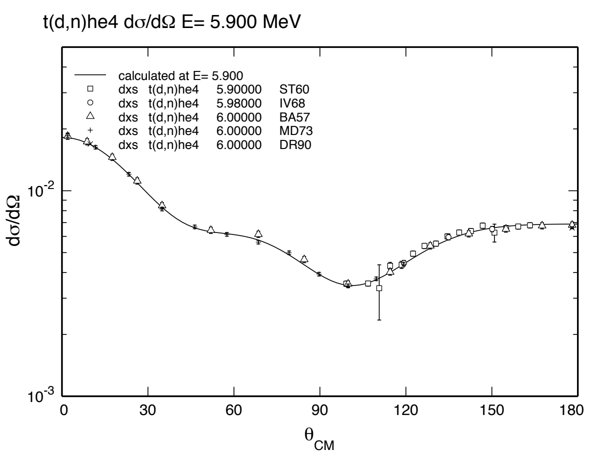


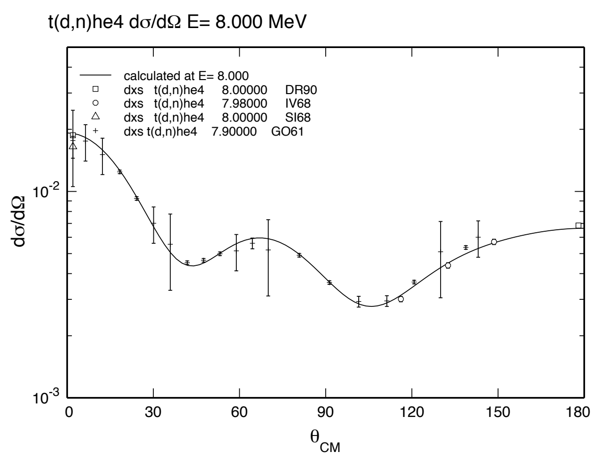
$^{3}H(d,n)^{4}He$ Differential Cross Section

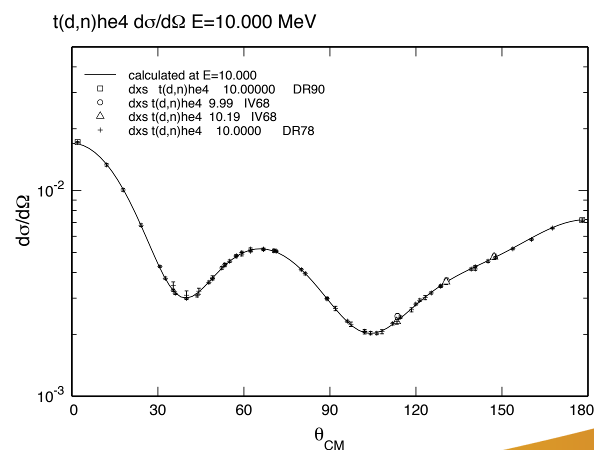




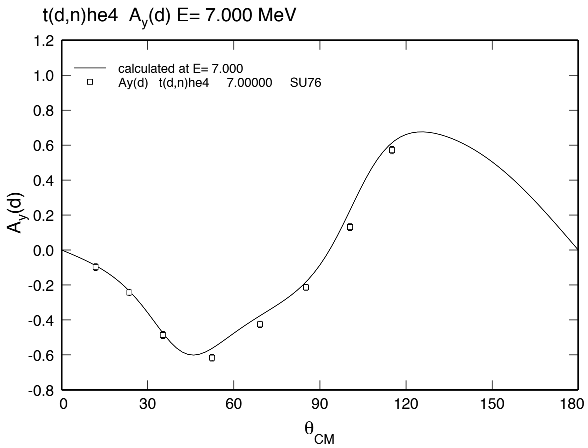


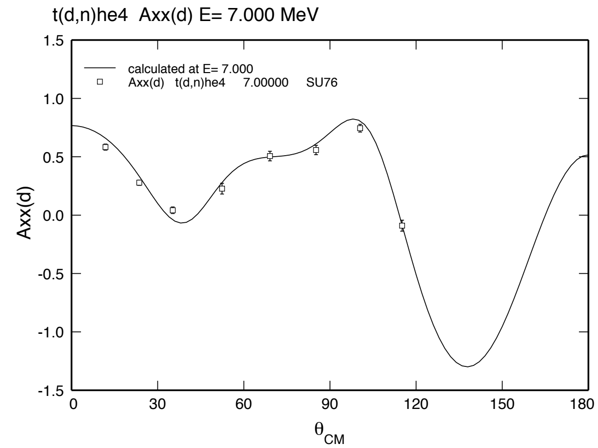


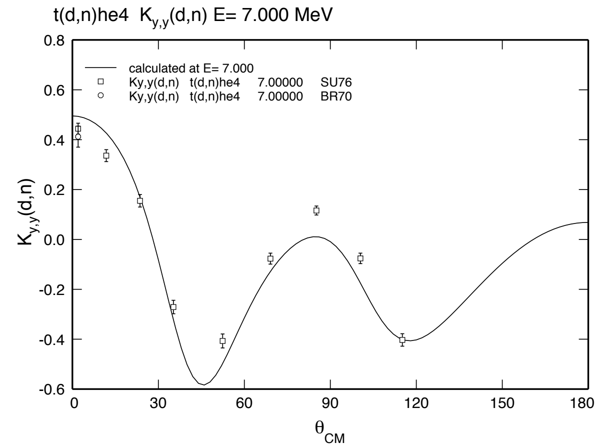


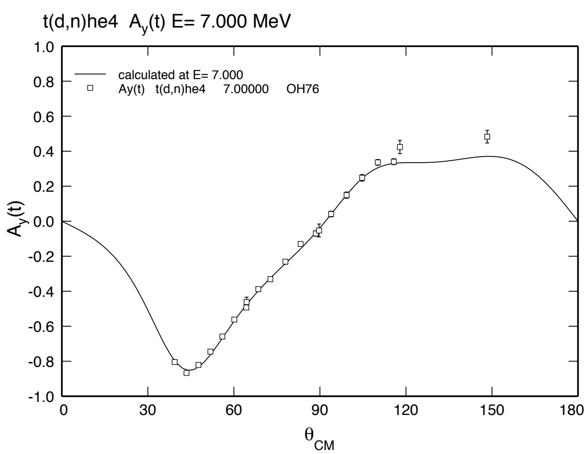


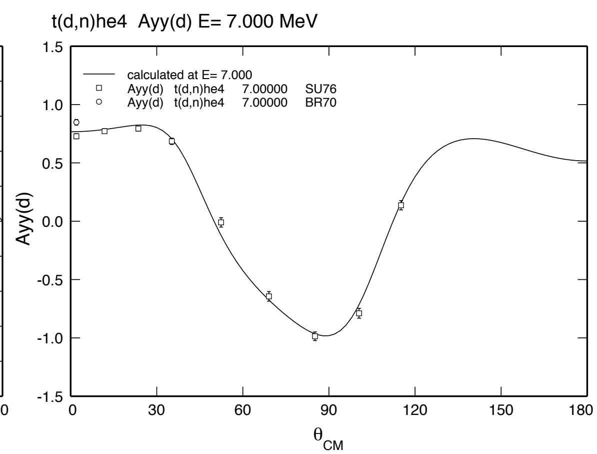
$^{3}H(d,n)^{4}He$ Polarizations at 7 MeV

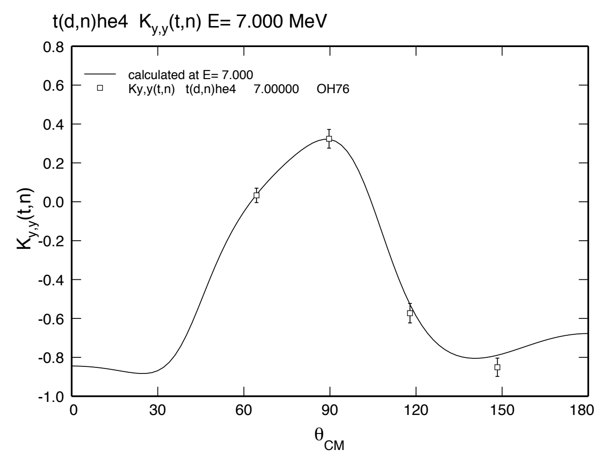




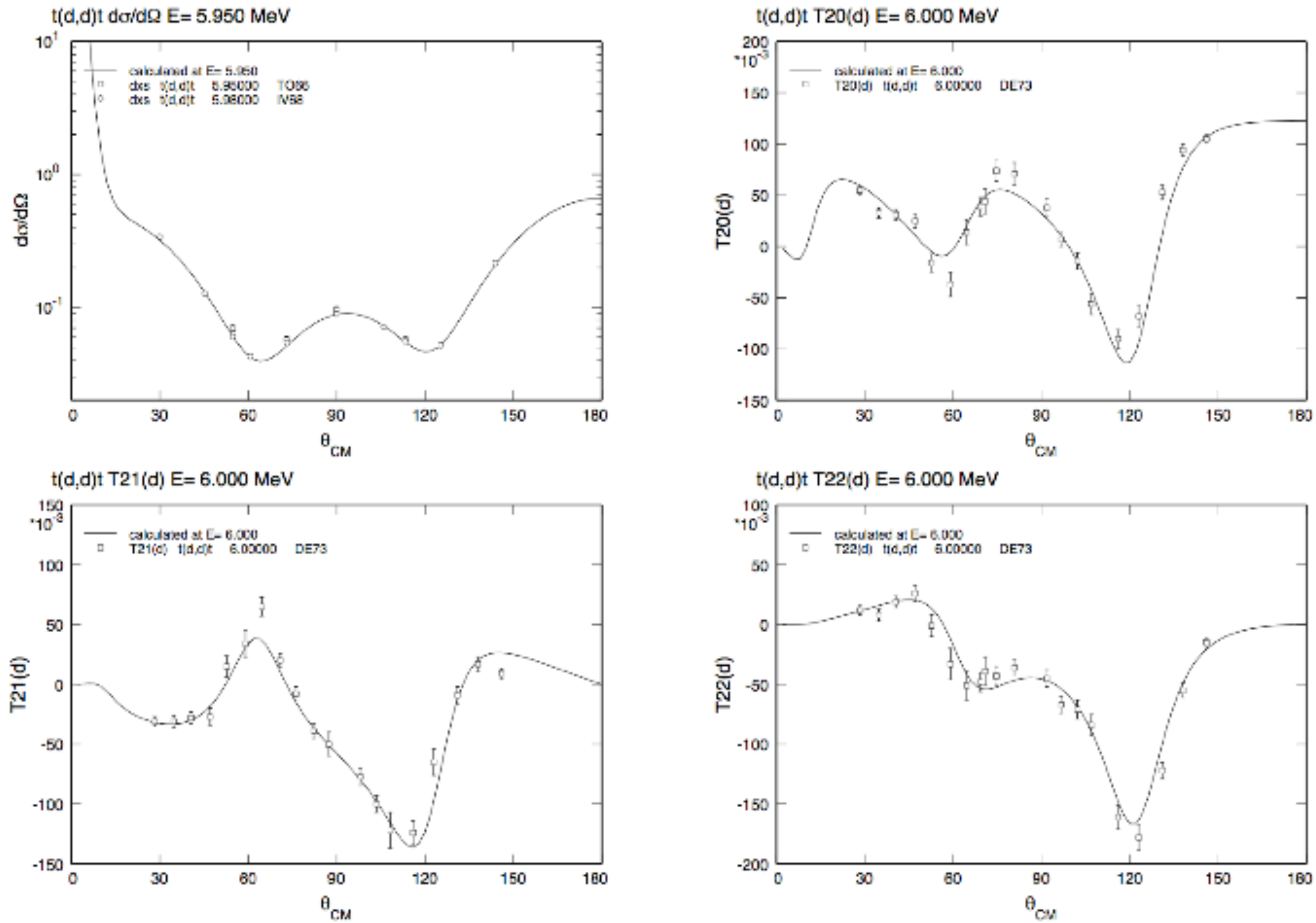








$^{3}H(d,d)^{3}H$ Observables at 6 MeV



Interaction with Wigner in 1975

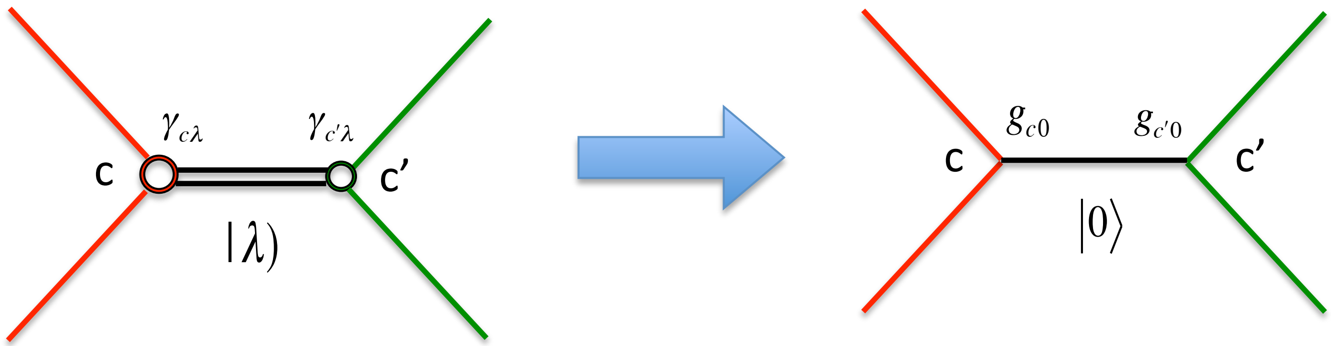
I met Eugene Wigner at the Conference on Nuclear Cross Sections and Technology (Washington, D.C.) in 1975.

He heard my talk about a coupled-channel *R*-matrix analysis of reactions in the ^{7}Li system, and was delighted that Don Dodder and I were applying the full capabilities of the framework to few-body reactions.

He also said:

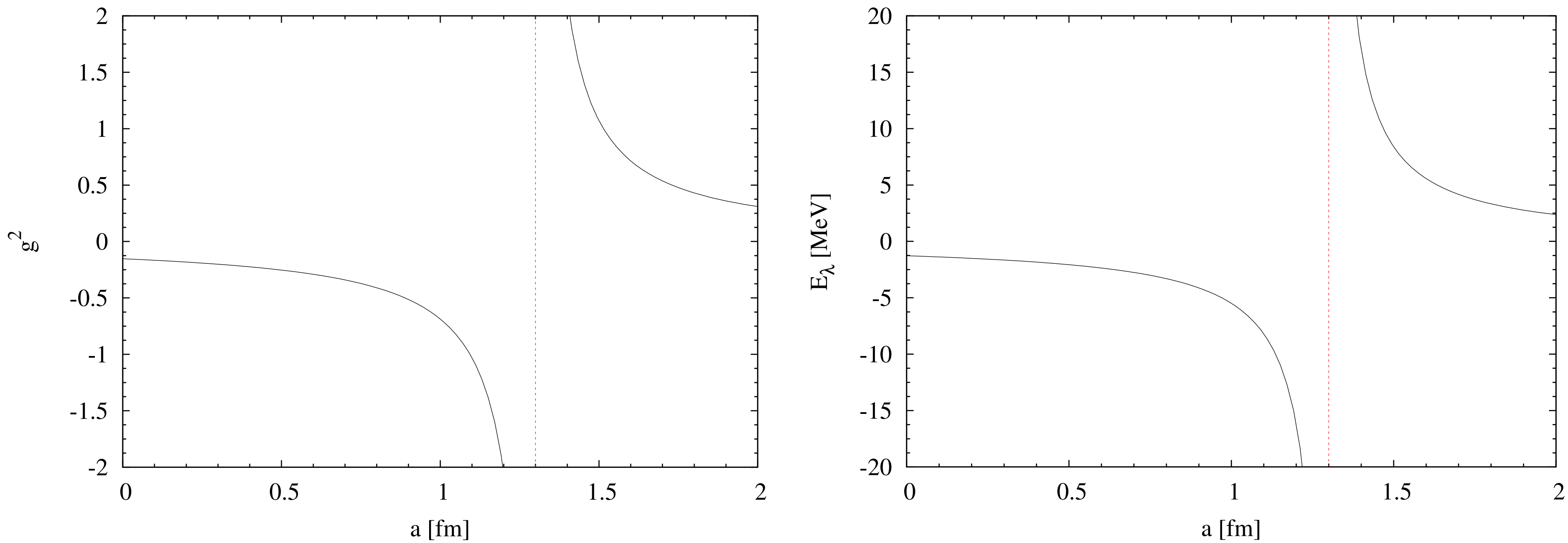
- I consider *R*-matrix theory to be my most important contribution to physics.
- I am thinking about what *R*-matrix theory looks like at zero channel radius.

R-Matrix and EFT



SL R-matrix Parameters at Small Radii

For singlet *n-p* scattering, we investigated the behavior of $g^2 = a\gamma_\lambda^2 / \hbar c$ and E_λ as a function of *a* for fixed values of a_0 = -23.7 fm and r_0 = 2.75 fm when they are obtained from $R(E) = \gamma_\lambda^2 / (E_\lambda - E)$:



The same sort of pole behavior in the *R*-matrix parameters was observed for triplet *n-p* scattering and for the *d+t* reaction as the channel radii were varied.

Summary and Outlook

- *R*-matrix theory contains all the basic requirements (unitarity, causality, and reciprocity) of the multi-channel scattering matrix in a simple pole expansion. It has proved to be the most successful phenomenological parametrization of experimental data available, and gives the correct continuation to complex energies (momenta).
- The presence of channel radii in the theory has been criticized by its detractors, but they are useful measures of the sizes of the interacting particles and the ranges of the strong forces between them. Asymptotic quantities in the theory (e.g., *T*) are independent of channel radii in principle, and their poles and residues do not depend on them in practice.
- Recent work shows that, although there are minimum channel radii at which R-matrix parameters are physical, they can be taken even to zero if the reduced width amplitudes are allowed to become pure imaginary, thereby establishing a connection with "wrong-sign" Lagrangians in effective field theory.
- Areas for more study: relativistic *R*-matrix forms, many-body breakup channels, explicit addition of direct effects (e.g., particle exchange), time-dependent *R*-matrix theory.