Covariances from Light-Element R-Matrix Analyses

G. M. Hale Theoretical Division (T-16) Los Alamos National Laboratory

- Summary of R-matrix formalism
- Implementation in EDA code
- Uncertainty propagation in EDA
- Examples: n+p, $n+^6Li$
- Possible extensions
- Conclusions

R-matrix Schematic

INTERIOR (Many-Body) REGION (Microscopic Calculations)



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,

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



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

Measurements

SURFACE

$$\mathcal{L}_{B} = \sum_{c} |c| (c) \left(\frac{\partial}{\partial r_{c}} r_{c} - B_{c} \right),$$

$$(\mathbf{r}_{c} | c) = \frac{\hbar}{\sqrt{2\mu_{c}a_{c}}} \frac{\delta(r_{c} - a_{c})}{r_{c}} \left[\left(\phi_{s_{1}}^{\mu_{1}} \otimes \phi_{s_{2}}^{\mu_{2}} \right)_{s}^{\mu} \otimes Y_{l}^{m}(\hat{\mathbf{r}}_{c}) \right]_{J}^{M}$$

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

Energy Dependent Analysis Code



Capabilities and Features

- 1) Accomodates general (spins, masses, charges) two-body channels
- 2) Uses relativistic kinematics and R-matrix formulation
- Calculates general scattering observables for 2→2 processes
- 4) Has rather general data-handling capabilities
- 5) Uses modified variable-metric search algorithm that gives parameter covariances at a solution.

Chi-square Expressions and Covariances

$$\chi^{2} = \sum_{i,j} (X_{i}(\mathbf{p}) - M_{i})(\mathbf{V}_{M}^{-1})_{ij}(X_{j}(\mathbf{p}) - M_{j}),$$
with $M_{i} = R_{i}S$, and $\mathbf{V}_{ij}^{M} = \underbrace{S^{2}(\Delta R_{i})^{2}\delta_{ij}}_{\text{diagonal piece}} + \underbrace{R_{i}R_{j}(\Delta S)^{2}}_{\text{rank-1 piece}}$ if R_{i} , S uncorrelated.
$$\chi^{2}_{\text{EDA}} = \sum_{i} \left[\frac{nX_{i}(\mathbf{p}) - R_{i}}{\Delta R_{i}} \right]^{2} + \left[\frac{nS - 1}{\Delta S/S} \right]^{2}$$

$$\rightarrow \chi^{2}_{0} + (\mathbf{p} - \mathbf{p}_{0})^{T}\mathbf{g}_{0} + \frac{1}{2}(\mathbf{p} - \mathbf{p}_{0})^{T}\mathbf{G}_{0}(\mathbf{p} - \mathbf{p}_{0})$$

The parameter covariance matrix is $C_0 = 2G_0^{-1}$, and so first - order error propagation gives

$$\begin{aligned} \operatorname{cov}[\sigma_{i}(E)\sigma_{j}(E')] &= \left[\nabla_{\mathbf{p}}\sigma_{i}(E)\right]^{\mathrm{T}}\mathbf{C}_{0}\left[\nabla_{\mathbf{p}}\sigma_{j}(E')\right]_{\mathbf{p}=\mathbf{p}_{0}} \\ &= \Delta\sigma_{i}(E)\Delta\sigma_{j}(E')\rho_{ij}(E,E') \\ \text{if } \mathbf{C}_{0} \rightarrow \varepsilon \mathbf{1}, \\ \tilde{\rho}_{ij}(E,E') &= \frac{\left[\nabla_{\mathbf{p}}\sigma_{i}(E)\right] \cdot \left[\nabla_{\mathbf{p}}\sigma_{j}(E')\right]}{\sqrt{\left[\nabla_{\mathbf{p}}\sigma_{i}(E)\right]^{2} \left[\nabla_{\mathbf{p}}\sigma_{j}(E')\right]^{2}}} \\ \end{aligned}$$

Convergence of EDA Solutions

Last 16 iterations of N-N(n-p) solution:

							$\sqrt{\mathbf{g}^{\mathrm{T}}\mathbf{g}}$				χ^2 /d.o.f.
it	1	hden	-1.62361E-06	fms	1.0000E+00	rmsq	2.799010E-01	time	160.444	WV	8.30020593E-01
it	2	hden	-2.70673E-07	fms	1.0000E+00	rmsq	5.057829E-02	time	172.095	WV	8.30020593E-01
it	3	hden	2.33652E-09	fms	1.0000E+00	rmsq	1.566784E-02	time	183.743	WV	8.30020593E-01
it	4	hden	-7.06336E-09	fms	1.0000E+00	rmsq	1.794353E-02	time	195.403	WV	8.30020593E-01
it	5	hden	1.46237E-11	fms	1.0000E+00	rmsq	1.492338E-02	time	207.047	WV	8.30020593E-01
it	6	hden	-4.36149E-08	fms	1.0000E+00	rmsq	3.261380E-02	time	218.701	WV	8.30020593E-01
it	7	hden	7.59279E-10	fms	1.0000E+00	rmsq	1.986385E-02	time	230.359	WV	8.30020593E-01
it	8	hden	-1.06823E-08	fms	1.0000E+00	rmsq	2.645074E-02	time	242.037	WV	8.30020593E-01
it	9	hden	1.19068E-10	fms	1.0000E+00	rmsq	2.243988E-03	time	253.693	WV	8.30020593E-01
it	10	hden	-1.85667E-10	fms	1.0000E+00	rmsq	3.034362E-03	time	265.350	WV	8.30020593E-01
it	11	hden	-1.07883E-12	fms	1.0000E+00	rmsq	2.767857E-03	time	277.018	WV	8.30020593E-01
it	12	hden	1.04047E-09	fms	1.0000E+00	rmsq	2.397856E-03	time	288.659	WV	8.30020593E-01
it	13	hden	2.24879E-12	fms	1.0000E+00	rmsq	2.951332E-03	time	300.303	WV	8.30020593E-01
it	14	hden	-2.08016E-09	fms	2.5000E-01	rmsq	4.356623E-03	time	317.050	WV	8.30020593E-01
it	15	hden	5.43813E-11	fms	6.5051E-01	rmsq	3.488838E-03	time	328.691	WV	8.30020593E-01
it	16	hden	-4.04937E-10	fms	1.0000E+00	rmsq	6.601823E-04	time	340.345	WV	8.30020593E-01

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

Channel	$a_{\rm c}({\rm fm})$	$l_{\rm max}$
<i>p+p</i>	3.26	3
n+p	3.26	3
$\gamma + d$	40	1

Reaction	# Pts.	χ^2	Observable Types
<i>p</i> (<i>p</i> , <i>p</i>) <i>p</i>	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	$\sigma_{\mathrm{T}}, \sigma(\theta), A_{y}(n), C_{y,y}, K_{y}^{y'}$
$p(n,\gamma)d$	80	133	$\sigma_{\rm int}, \sigma(\theta), A_{\rm v}(n)$
$d(\gamma,n)p$	59	35	$\sigma_{\rm int}, \sigma(\theta), \Sigma(\gamma), P_{\rm v}(n)$
Norms.	129	72	
Total	5338	4287	19

free parameters = $44+129 \Rightarrow \chi^2/\text{degree of freedom} = 0.830$

n-p Scattering Lengths

From the analysis,

 $a_0 = -23.719(5)$ fm, $a_1 = 5.414(1)$ fm, giving $a_0 = (3a_1 + a_0)/4 = -1.8693$ fm,

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

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

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 AV18 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



Summary of ⁷Li Analysis

Channel	$a_{c}(fm)$	l _{max}
<i>t</i> + ⁴ He	4.02	5
<i>n</i> + ⁶ Li	5.0	3
$n+{}^{6}\text{Li}^{*}$	4.5	1

Reaction	Energy Range	# Pts.	$\chi^2/Pt.$
$^{4}\text{He}(t,t)^{4}\text{He}$	$E_t = 0.14 \text{ MeV}$	1622	0.930
4 He(<i>t</i> , <i>n</i>) 6 Li	$E_t = 8.75 - 14.4 \text{ MeV}$	35	1.658
$^{4}\text{He}(t,n)^{6}\text{Li}^{*}$	$E_t = 12.9 \text{ MeV}$	3	2.964
$^{6}\text{Li}(n,t)^{4}\text{He}$	$E_n = 0.4 \text{ MeV}$	860	1.039
$^{6}\text{Li}(n,n)^{6}\text{Li}$	$E_n = 0.4 \text{ MeV}$	798	1.391
Total	χ^2 /d.o.f.	3318	1.164

t-⁴He Scattering



⁶Li(n,t) Cross Section



Covariances for ⁶Li(*n*,*t*) Cross Sections



"Pure Theoretical" Correlations?





Summary/Conclusions

- R-matrix approach is ideal for obtaining detailed covariances for light-element reactions, but not always over the full energy range desired.
- Implementation in EDA gives accurate covariance information (assuming that relative and absolute values of measured data are determined independently) from first-order error propagation for all reactions.
- "Pure theoretical" correlations from microscopic calculations may be useful for extending R-matrix covariances to higher energies.