Recent Advances in R-matrix Data Analysis

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R-matrix Theory

- The theory to describe individual resonances in A+B scattering, and the non-resonant background between them.

- Describes all the asymptotic properties of the A+B wave function outside some fixed radius, \( R \geq a \), in terms of pole energies \( e_p \) and reduced width amplitudes \( \gamma_{np} \) for each channel \( n \) and pole \( p \).
  - The \( \gamma_{np} \) are calculated from structure theory, or
  - or the \( \gamma_{np} \) are fitted to scattering data

- The basis for making statistical approximations
  - Reich-Moore approximation
  - Hauser-Feshbach models, etc.

- Basis for checking the accuracy of those models.
Foundation of R-matrix theory: ‘Lane and Thomas’

**R-matrix Theorem:**
For Hermitian $H = T + V + B$ with Bloch operator $B$, with $V \neq 0$ only for $r \in [0,a]$ and $E$-independent, then the exact scattering solution $H\Psi = E\Psi$ can be represented by a R-matrix at $r=a$ with a set of pole energies $e_p$ and reduced width amplitudes $\gamma_{np}$ as

$$ R_{mn}(E) = \sum_{p=1}^{\infty} \frac{\gamma_{mp} \gamma_{np}}{E - e_p} $$

**R-matrix Practice:** use finite number $N$ of poles $p$: $\sum_{p=1}^{N}$
We can obtain useful converged results with ‘background poles’.

- Both exact and practical R-matrices:
  1. Yield unitary S-matrix at each energy
  2. Yield orthogonal scattering wave functions at different energies.
Any proposed extension only accepted if at least
1. Yields unitary $S$-matrix at each energy
2. Yields orthogonal scattering wave functions at different energies.

Both conditions derive from a Hermitian and energy-independent Hamiltonian.

Reich-Moore approximation: imaginary damping widths for missing channels:
   — Condition 1. not satisfied e.g. if imaginary damping terms: Reich-Moore
     • Perhaps ok if a specific meaning is given to the missing flux, e.g. capture or fusion

Convenient changes to boundary conditions in the Bloch operator:
   — Condition 2. not satisfied e.g. boundary condition $B$ not constant: $B=S(E)$
   — Conditions 1,2 are satisfied in the Brune basis (transformable to/from L&T!)
Verification of R-matrix Codes

- IAEA (Vienna) has had a series of consultants meetings since 2015 to improve R-matrix modeling accuracy and ranges of applications.
- Improve for neutron and charged-particle reactions.
- Verify codes
  Compare search procedures
  Validate R-matrix data fits.

- Codes participating:
  - ORNL: SAMMY
  - LLNL: FRESCO
  - LANL: EDA
  - JAEA: AMUR
  - Notre Dame: AZURE2
  - Future confirmation:
    - CEA: CONRAD
    - Tsinghua: RAC

- I have written ‘ferdinand.py’, to translate between most of the input-output formats.
  - Uses GNDS intermediate structure.

Recent meeting: https://www-nds.iaea.org/index-meeting-crp/CM_R-matrix2018/
Examples: $^4\text{He}+^3\text{He}$ elastic scattering with $p+^6\text{Li}$
Find R-matrix fit.

Dominant channels: $^4\text{He}+^3\text{He}$ and $p+^6\text{Li}$
Next: $p_1+^6\text{Li}^*$ ($p_1=3^+, p_2=2^+$, etc) breakup.

Selected data to be fit up to 8.0 MeV $^7\text{Be}^*$ excitation

<table>
<thead>
<tr>
<th>Channels</th>
<th>Data points</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a,a)</td>
<td>1609</td>
</tr>
<tr>
<td>(a,p)</td>
<td>120</td>
</tr>
<tr>
<td>(p,a)</td>
<td>630</td>
</tr>
<tr>
<td>(p,p)</td>
<td>420</td>
</tr>
</tbody>
</table>

Figure 1: Level diagram of $^7\text{Be}$. The low mass nucleus has only two bound states, the ground state and the level at $E_x = 0.429$ MeV.

- The 9.206 MeV point at 36.999 deg in the Spiger $aa$ data was erroneously digitized on EXFOR. The point has been removed.
- The Tombrello $aa$ data have an additional digitization error of 0.5 mb/sr, this has been added in quadrature to the percent errors for the A1295002 EXFOR data.
- The Lin $pa$ data that James sent us was converted by him from cm data. Ian's checks, however, show that in 3 cases of angles near 90 deg, James chose the wrong quadrant. This has been corrected.
- The Spiger $aa$ data of A1094006 has a 0.08 MeV digitization error. Ian finds that the data are much more consistent with the other data sets if they are translated in energy by 0.1 MeV.

References

Example: R-matrix fit $^4\text{He}+^3\text{He}$ scattering.

1. Barnard_aa data

Search file: test1b-v9gL-xs2.sfrescoed+.sfresco;

Dataset | Chisq/pts av norm
---|---
Barnard_aa.dat | 0.967 0.990

Experiment/R-matrix ratios

data_Barnard_aa.dat_1-7-9gL-xs2.agr (spacing 0.2)
Most codes agree within 1% to AMUR.

0.1% agreement would be better.

Here only away from the 7 MeV resonance.
(or maybe AMUR code is poor.)

RAC not agreeing.
R-matrix fit of Spiger_aa data (more $^4$He+$^3$He)

Search file: test1b-v9gL-xs2.sfrescoed+.sfresco;

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Chisq/pts av norm</th>
<th>av shift</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spiger-A1094004-lab_aa.dat</td>
<td>2.633</td>
<td>0.929</td>
</tr>
</tbody>
</table>

data_Spiger-A1094004-lab_aa.dat_8-21-9gL-xs2.agr (spacing 0.2)
Brune basis: matches resonances in phase shifts

- Original fit done with $B=-L$ boundary conditions. But can reversibly transform to the Brune basis.

<table>
<thead>
<tr>
<th>$B=-L$ Brune basis</th>
<th>$J^\pi=3.5^-$ cm:</th>
<th>$-12.499$ to $2.975$ MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$J^\pi=2.5^-$ cm:</td>
<td>$6.236$ to $5.033$ MeV</td>
</tr>
<tr>
<td></td>
<td>$J^\pi=2.5^-$ cm:</td>
<td>$7.058$ to $5.593$ MeV</td>
</tr>
</tbody>
</table>

Historically, the $B=S(E)$ approximation was used to give R-matrix pole energies close to the observed resonances. But this approximation gives different background between poles.
Extensions to higher energies?

- At high incident energies, there are more and more inelastic or transfer two-body channels.
  - Numbers of partial waves increase, but still standard theory.

- At higher energies, breakup channels begin to open.
  - Normally three-body channels, and more difficult to model
  - Maybe approximate by cascaded two-body channels.

- Alternatively, we could settle for damping widths $\Gamma_p$ to describe loss of flux to outside the model space (an ‘optical’ R-matrix model):
  \[
  R_{mn}(E) = \sum_{p=1}^{\infty} \frac{\gamma_m \gamma_n}{E - e_p + i\Gamma_p/2}
  \]

- This could be allowed if there are specific physical channels missing from the model (never for bound states).
An ‘optical’ R-matrix model?

- Alternatively, we could settle for damping widths $\Gamma_p$ to describe loss of flux to outside the model space like an optical model:

$$R_{mn}(E) = \sum_{p=1}^{\infty} \frac{V_{mp}V_{np}}{E-e_p+i\Gamma_p/2}$$

- Inspired by “Reduced R-matrix” theory of Lane & Thomas (1958, ch. X).
- Using approximations like Reich-Moore but for particles, as begun in RAC

- This could be allowed if there are specific physical channels missing from the model (never for bound states).
  - Then the missing flux (from the unitarity defect) could (for example) be fed into a Hauser-Feshbach decay model built only on the missing physics

- But if the total width of a damped resonance is large, then the flux will start missing at lower energies, even below the known threshold for the excluded channels!
Example of fitting damping widths:
Redo $^4\text{He}+^3\text{He}$ elastic scattering without $p+^6\text{Li}$

- Fits data rather well,
  - though $\chi^2 / df = 7.32$

- But absorption still present below 10 MeV: unphysical.
Energy-dependent Damping Widths?

- A simple proposal to include the known energy dependence of flux going to an excluded channel with known threshold $E_0$.

- Make the damping width energy-dependent: $\tilde{\Gamma}_p(E)$
  - Make energy dependence behave as $\Gamma = 2\gamma^2 P_L(E)$ like R-matrix widths
  - So choose
    $$\tilde{\Gamma}_p(E) = \tilde{\Gamma}_p \frac{P_L(E - E_0)}{P_L(e_p - E_0)}$$
  - This cuts off the damping for $E \leq E_0$, and gives $\tilde{\Gamma}_p(e_p) = \tilde{\Gamma}_p$ to be fitted.

- Making this work depends on
  - Having good data for angular distributions above the $E_0$ threshold
  - May need to choose $e_p$ energy in the Brune basis for best physics
  - Knowing physics of missing channels to estimate $L$ and Coulomb barriers
    - For exit in $M$-body hyper-spherical harmonic $K$, use $L = K + (3M - 6)/2$
Example fit with Energy-dependent damping

Refit $^4\text{He} + ^3\text{He}$ data. Choose $e_p$ energy in the Brune basis, with $L = 0$, $E_0 = 4.02$ (MeV).

Result: $\chi^2 / df = 4.25$

Search file: test1b-v9gL-aa10.sfrescoed;

First attempt at least gives average transfer cross-sections