

FRESCO: Coupled-channels Calculations

*Finite-Range with **Exact Strong CO**uplings.*

Talk at INT 15-58W, Seattle

Wed, March 4, 2015

Ian Thompson



LLNL-PRES-667633

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC



Fresco

- Started in 1983 at Daresbury Laboratory
- First for 2-step transfer contributions to $^{17}\text{O}^*$.
- Main paper in 1988: *Computer Physics Reports*, Vol 7, 167-212. Now has 930 citations.
- Source & docs available at www.fresco.org.uk, hosted at Univ. Surrey.
- Versions since 2006: ‘public’ FRES (3.1), and ‘Livermore’ FRXY (6l) ✕
- Textbook (CUP, 2009) “*Nuclear Reactions for Astrophysics*” with Filomena Nunes. Now sold 873 copies.
- Still being maintained, and developed, with queries answered.

2-step transfer contributions to $^{17}\text{O}^*$

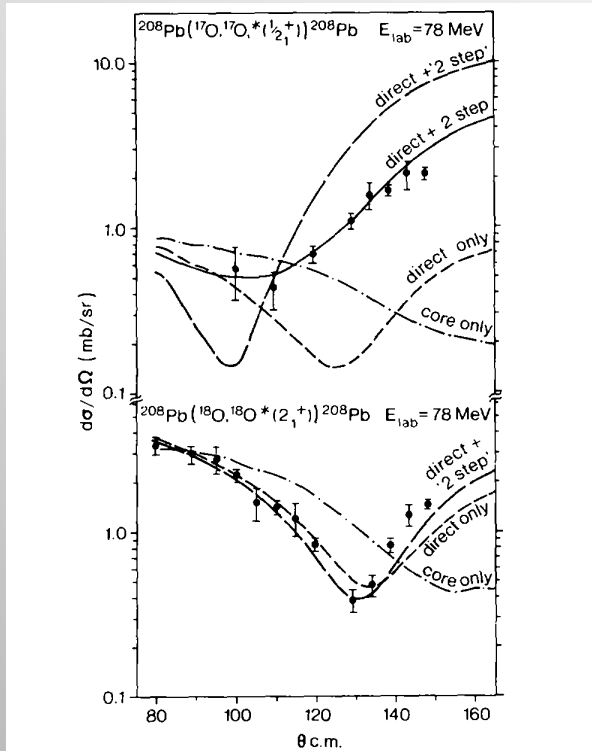


Fig. 2. Differential cross section measurements of the $^{208}\text{Pb}(^{17}\text{O}, ^{17}\text{O}^*(1/2^+))^{208}\text{Pb}$ (upper) and the $^{208}\text{Pb}(^{18}\text{O}, ^{18}\text{O}^*(2^+))^{208}\text{Pb}$ (lower) reactions at 78 MeV incident energy. The curves are theoretical calculations. The dot-dashed curve includes Coulomb excitation and the nuclear core (^{16}O) excitation only. Adding the valence neutron interaction gives the short-dashed ("direct only") curve. The effect of adding two-step transfer processes using the approximations of ref. [1] is given by the long-dashed curve; the solid curve is the result of a more rigorous calculation described in the text.

Lilley et al, PL 128B, 153 (1983)

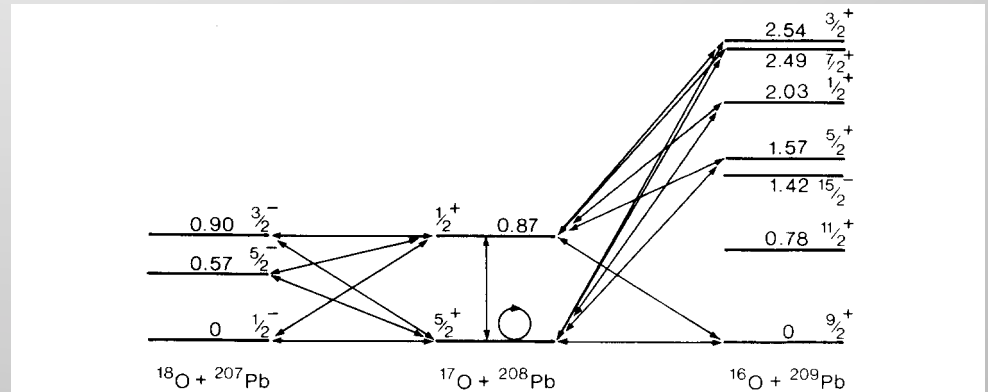


Fig. 6. Channel couplings used in the multistep CRC calculations of the $^{17}\text{O}-^{208}\text{Pb}$ interaction at 78 MeV.

Lilley et al, NPA 463, 710 (1987)

Documentation

- *Methods of Direct Reaction Theories*, paper in “Scattering” ed. Pike & Sabatier (2001)
- *User Guide: Appendix A of Nuclear Reactions for Astrophysics*(2009)
- *Coupled Channels Methods for Nuclear Physics*, (1988)
- Input manual

See <http://www.fresco.org.uk/documentation.htm>

Basic Idea

- Reactions between two nuclei: entrance and exit
- Multiple mass partitions.
- Energy, spin and parity given for all initial and final states of all nuclei.
- Unlimited lists of potentials and couplings.
- Solve coupled equations
- Predict cm cross section distributions.
- Standard forms for
 - optical potentials,
 - bound states,
 - inelastic, transfer and capture mechanisms,
 - etc
- Written in Fortran 90
 - Tested on wide range of compilers

The Coupled Equations

For each total spin J_{tot} and parity π

$$[T_{xL}(R) + V_c(R) - E_{xpt}] \psi_\alpha(R) + \sum_{\alpha'} \langle \alpha | V | \alpha' \rangle \psi_{\alpha'}(R') = 0.$$

with

$$\hat{T}_{xL}(R_x) = -\frac{\hbar^2}{2\mu_x} \left[\frac{d^2}{dR_x^2} - \frac{L_x(L_x+1)}{R_x^2} \right]$$

and

$$\langle \alpha | V | \alpha' \rangle \quad \text{either local } R=R', \text{ or non-local } R \neq R'$$

satisfying the boundary conditions

$$\psi_{\alpha\alpha_i}^{J_{\text{tot}}\pi}(R_x) = \frac{i}{2} \left[H_{L_i}^-(\eta_\alpha, k_\alpha R_x) \delta_{\alpha\alpha_i} - H_L^+(\eta_\alpha, k_\alpha R_x) \mathbf{S}_{\alpha\alpha_i}^{J_{\text{tot}}\pi} \right]$$

Optical and Binding Potentials

- Central, spin-orbit and tensor forces.
 - WS, Gaussian (etc) shapes, or read in.
 - Deformation by rotational model, or by arbitrary strengths
 - Linear energy interpolations.
- ✘ L-, J-, and parity-dependent potentials.
 - ✘ Effective masses $m^*(r)$
 - ✘ Lane isospin couplings

Coupling Mechanisms

- Inelastic
 - Deformed optical pots.
 - Single-particle excitations
- Transfers of a cluster
 - Zero range, LEA.
 - Finite range
 - Non-orthogonality terms.
- Two-nucleon transfers
 - From & to correlated 2N wfs from correlated 1N wfs, or read in from 3-body code.
 - Sequential and Simultaneous
- Capture to γ channels
 - E_k in Siegert approx.
 - M_k magnetic transitions
 - (both in localized approx.)
- R-matrix phenomenology
- General LSJ couplings
 - Local or non-local
 - Numerical forms read in
- ✕ General partial wave couplings
 - Numerical local or nonlocal

Solving the Coupled Equations

- Numerov integration of equations with local couplings: 'exact'
- Iteration on non-local couplings (eg. transfers).
- Use Pade acceleration if n -step DWBA diverges.
- Use James Christley's coupled-Coulomb wave functions CRCWFN for long-range multipoles
- Isocentrifugal approx.
- R-matrix solutions:
 - Expand on eigenstates of diagonal optical pots
 - Need Buttle corrections.
 - More stable numerically
- ✘ Lagrange-mesh method:
 - From Daniel Baye (ULB)
 - No Buttle correction needed
- ✘ MPI: to solve J^π sets in parallel.
- ✘ OPENMP: to solve coupled equations for given J^π .

Breakup: beyond 2-body channels

■ CDCC:

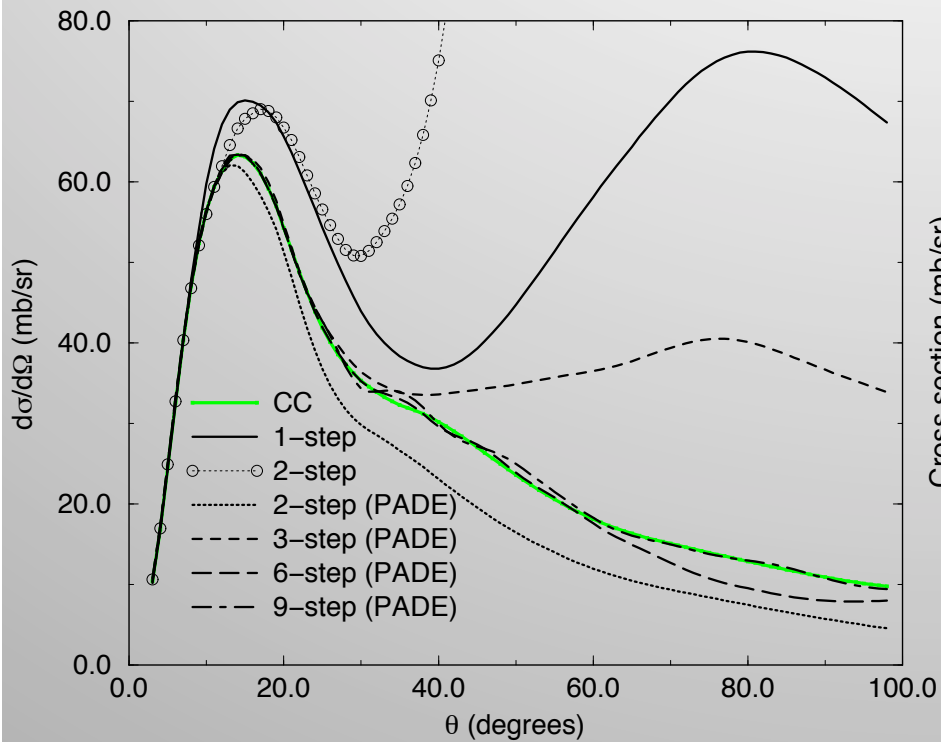
- Use continuum single-particle states
- Orthonormalized in segments.
- Post-processing by Jeff Tostevin for coincidence breakup cross sections.
- Converges ok (if no transfer bound states!)

✕ XCDCC

- Neil Summers extended CDCC method to deal with deformed core states in single-particle states.
- Example for breakup of $^{11}\text{Be} = ^{10}\text{Be}(0^+, 2^+) + n$

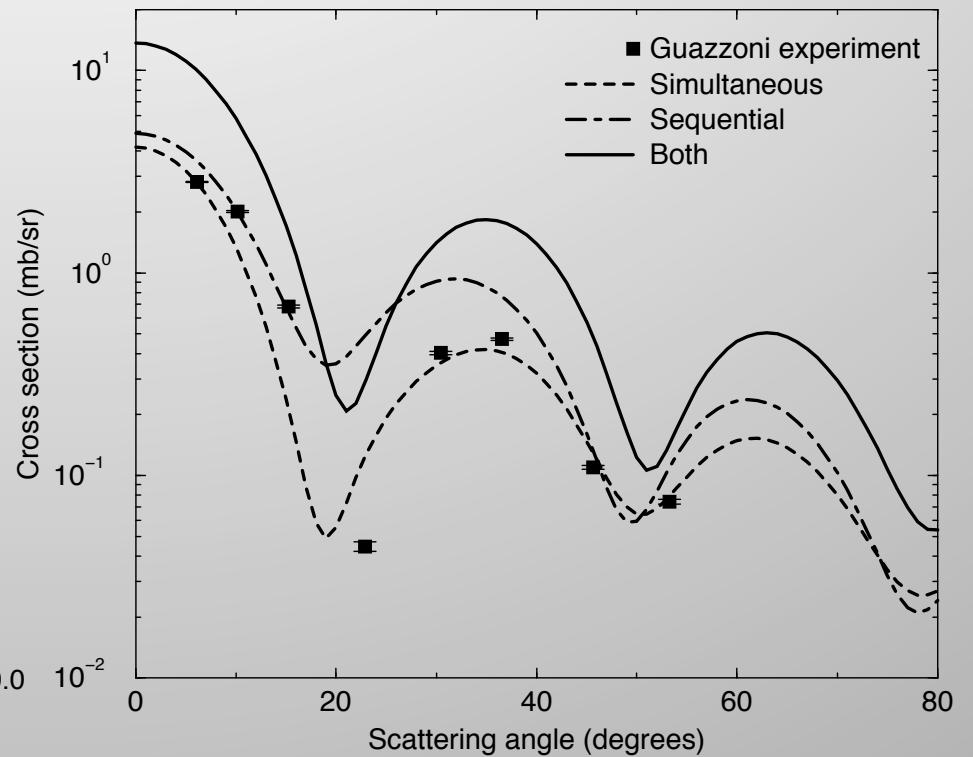
Coherent multistep effects

$^8\text{B} + ^{58}\text{Ni}$ breakup at 26 MeV



Nunes & Thompson, PRC 59, 2652 (1999)

$^{124}\text{Sn}(p,t)$ at 25 MeV



Thompson, in Broglia et al (2013)

Input Formats

- OLD style #1:
 - Card inputs cols 1—72
- NAMELIST style #2:
 - Fortran var=value text
- CDCC style #3:
 - Generate easily the NAMELIST sets of bins and couplings for CDCC calculations.

Output Formats

- Cross sections $\sigma(\theta)$
- Amplitudes $f_{mM:m'M'}(\theta)$
- CDCC amplitudes for post-processing.

Sfresco: searching for χ^2 minimums

- Define data with errors:
 - Energy and/or angle data
 - Polarization data
 - Angle-integrated data
 - Phase shifts in given channel
 - Fitted bound state parameters
- Define parameters
Initial values and limits of:
 - Optical parameters
 - Spectroscopic amplitudes
 - R-matrix pole energies & widths
 - Data normalizations
- Searching
 - Interactive or given method
 - Uses MINUIT
 - Plot initial or final fits
 - Trace χ^2 progress
 - Restart at any trial set.

Current Developments

✂ LLNL:

- General nonlocal potentials
- Effective masses $m^*(R)$
- Lane couplings for IARs
- IAR non-orthogonality (p, p')
- Semi-direct capture step
- Surface operator for transfer

■ Jeff Tostevin:

- Breakup coincidence cross sections with core excitation in XCDCC
- Simple zero-range transfers

■ Alex Brown

- Using shell-model two-nucleon overlaps for transfers (seq+sim).

■ Antonio Moro:

- Stabilizing the solutions from Numerov method
- More NN standard forms for tensor forces
- Deformations in optical potentials in transfer operator

Missing Capabilities

- Core transitions in electromagnetic particle steps.
- Perey-Buck nonlocality in optical potentials.
- Spin-dependence of optical potentials in transfer operators.
- Energy-dependence of optical potentials in transfer operators.
- Uniform treatment of antisymmetrization and identical particles
- Convergence problems: CDCC breakup with all-order couplings to transfer channels.



**Lawrence Livermore
National Laboratory**