FRESCO: Coupled-channels Calculations

*Finite-Range with Exact Strong COuplings.*

Talk at INT 15-58W, Seattle
Wed, March 4, 2015

Ian Thompson
Fresco

- Started in 1983 at Daresbury Laboratory
- First for 2-step transfer contributions to $^{17}\text{O}^*$.
- Source & docs available at [www.fresco.org.uk](http://www.fresco.org.uk), hosted at Univ. Surrey.
- Versions since 2006: ‘public’ FRES (3.1), and ‘Livermore’ FRXY (6l)
- Still being maintained, and developed, with queries answered.
2-step transfer contributions to $^{17}$O$^*$


Lilley et al, NPA 463, 710 (1987)

Fig. 2. Differential cross section measurements of the $^{208}$Pb ($^{17}$O, $^{17}$O$^*$(1/2$^+$))$^{208}$Pb (upper) and the $^{208}$Pb ($^{18}$O, $^{18}$O$^*$(2$^+$)) $^{208}$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.

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

- Input manual

See [http://www.fresco.org.uk/documentation.htm](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 $\pi$

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

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

$$\langle \alpha | V | \alpha' \rangle \quad \text{either local } R=R', \text{ or non-local } R\not=R'$$

satisfying the boundary conditions

$$\psi_{J_{tot}^{\pi}}(R_x) = \frac{i}{2} \left[ H^{-}_{L_i}(\eta_\alpha, k_\alpha R_x) \delta_{\alpha \alpha_i} - H^{+}_{L_i}(\eta_\alpha, k_\alpha R_x) S^{J_{tot}^{\pi}}_{\alpha \alpha_i} \right]$$
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 potls.
  - 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 $\gamma$ 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 potls
  - Need Buttle corrections.
  - More stable numerically
- Lagrange-mesh method:
  - From Daniel Baye (ULB)
  - No Buttle correction needed
- MPI: to solve \( J^\pi \) sets in parallel.
- OPENMP: to solve coupled equations for given \( J^\pi \).
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

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

Nunes & Thompson, PRC 59, 2652 (1999)

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 $\chi^2$ 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 $\chi^2$ 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.