united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

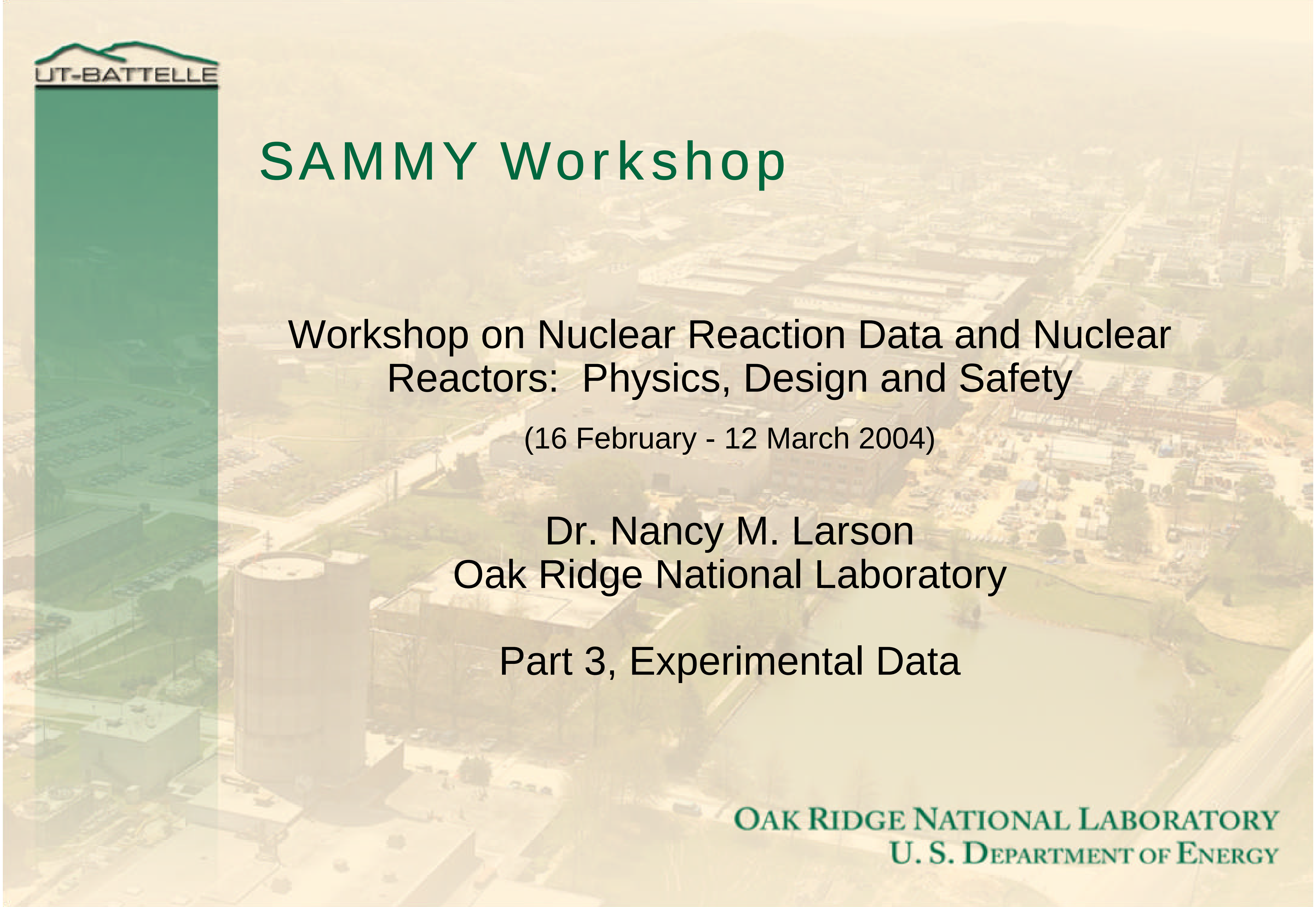
SMR.1555 - 29

Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety

16 February - 12 March 2004

Further on SAMMY (I)

Nancy M. LARSON
Oak Ridge National Laboratory
Building 5700 MS 6171
P.O. Box 2008
TN 37831-6171 Oak Ridge
U.S.A.



UT-BATTELLE

SAMMY Workshop

Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

(16 February - 12 March 2004)

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 3, Experimental Data

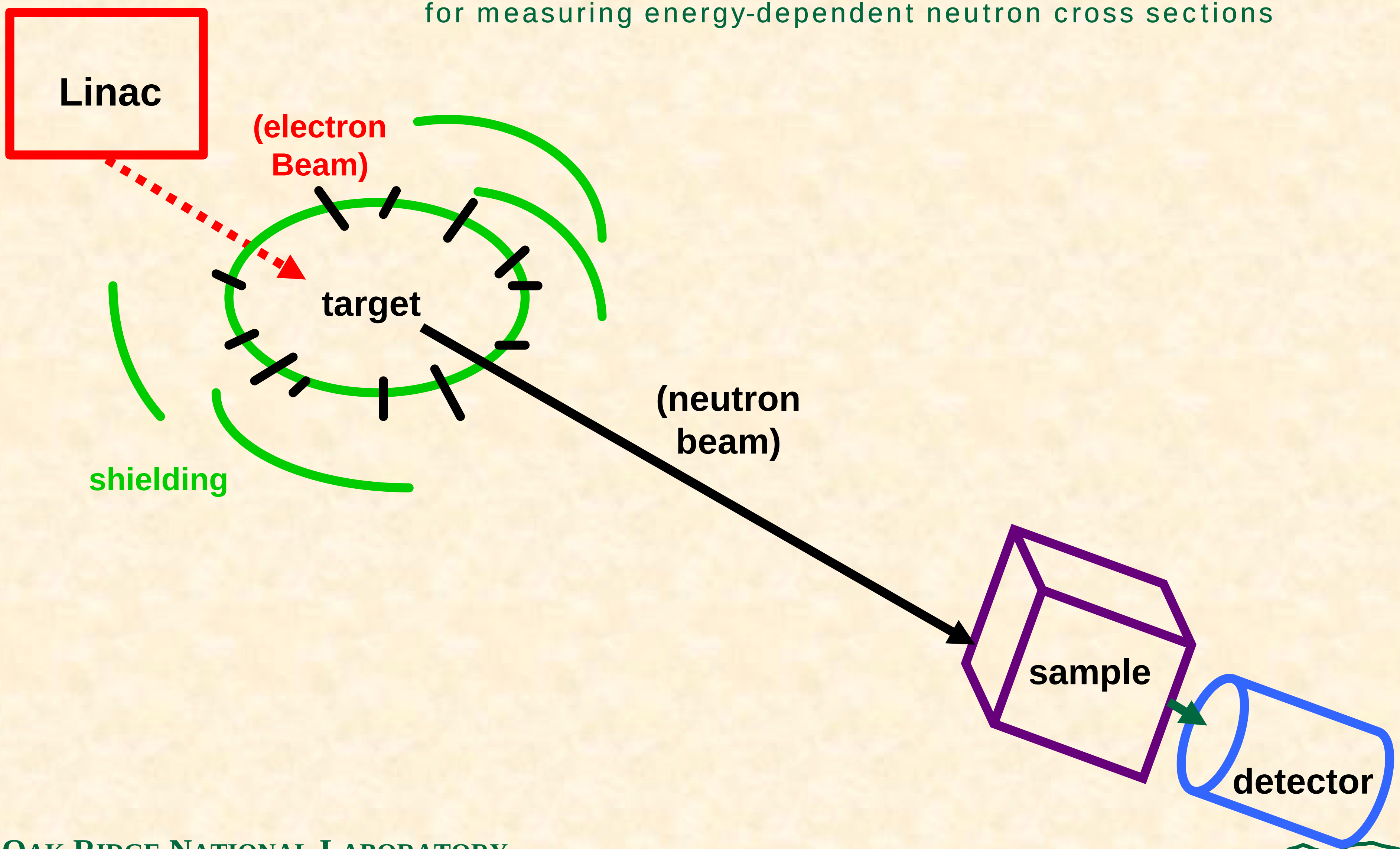
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Why do we care about cross sections?

- **Fundamental physics**
  - **Humans are curious about everything**
- **Practical applications**
  - **So we can calculate when a reactor would go critical, or how much shielding is needed**
  - **Medical needs**
  - **Nuclear astrophysics / stellar evolution**

Time of Flight Experiment

for measuring energy-dependent neutron cross sections



What do we learn from time-of-flight?

- **Measure path length *L* precisely**
- **Know time t_0 at which neutron leaves target**
  - **because beam is pulsed**

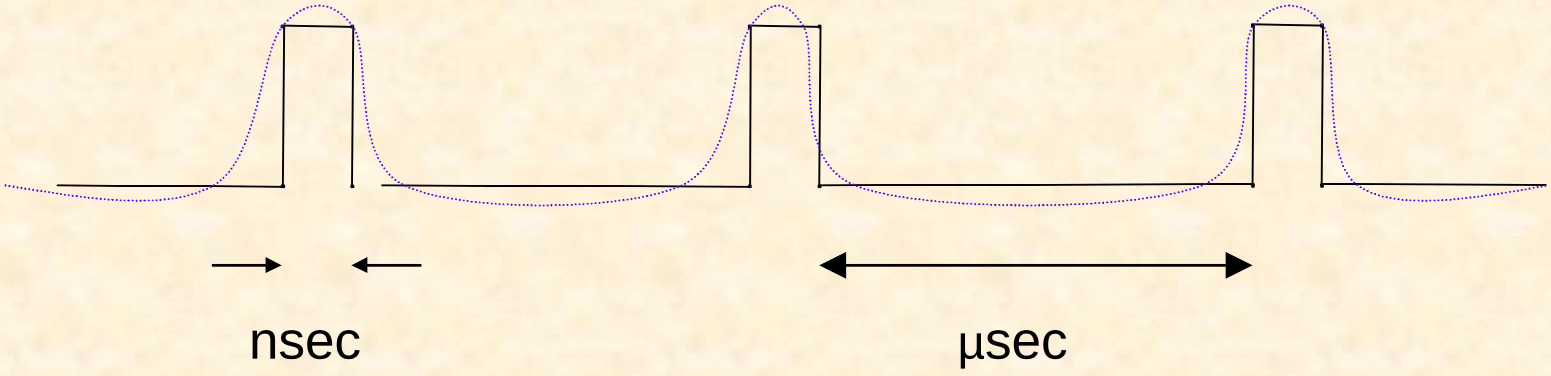
or proton, or fission fragment, or whatever

- **Find time *t* at which neutron reaches detector**
- **Therefore know energy *E*:**

$$E = \frac{m}{2}\left(\frac{L}{\left(t - t_0\right)}\right)^2$$

***Data* are “number of counts reaching detector” vs “time” (i.e. vs “energy”)**

Linac e- beam



Pulse width

Repetition rate

These will change from site to site, and from experiment to experiment. Likewise, pulse shape will change.

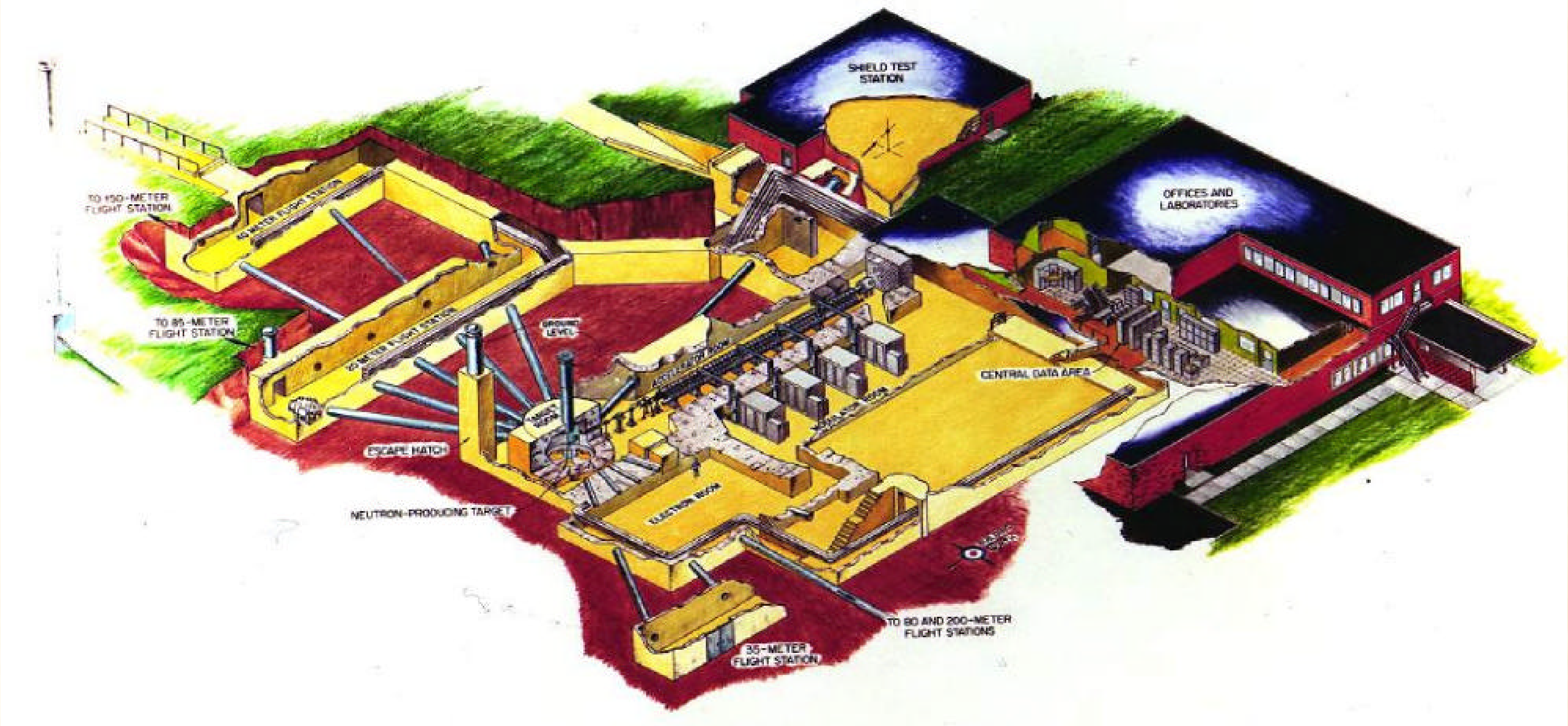
Target composition –

Ta + H_2O at ORELA at Oak Ridge, TN, USA
^{235}U at GELINA at Geel, Belgium
Pb at CERN in Geneva, Switzerland

To summarize: time of flight experiments measure energy-dependent neutron cross sections as follows:

- An accelerator produces a beam of electrons. (Usually this is a linear accelerator such as the Oak Ridge Electron Linear Accelerator (ORELA), the Geel LINAC (GELINA), or the Gaerttner LINAC at Rensselaer Polytechnic Institute.)
- The electrons hit a target (water and tantalum at ORELA, Uranium at GELINA).
- This produces neutrons, which fly straight outward in all directions. Shielding and collimators are used to collimate the beam.
- The neutrons are used as a probe to study nuclei. Samples of the material to be studied are placed in the beam line where neutrons will interact with nuclei in the sample.
- Detectors literally count the particles that reach them.
- Experimentalists "reduce" the "count" to a quantity which resembles a "cross section." This data-reduction process involves dead-time corrections, background subtraction, normalization, and many other operations.
- The next step is to interpret the results in terms of phenomenological scattering theory (R-matrix theory). *The major emphasis of this class will be on this step.*

The ORELA Facility



ORELA Facility Details

- Electron energy 180 MeV maximum
- Peak Current 20 amps maximum
- Power on target 60 kW maximum
- Electron beam diameter 1 cm
- Neutron targets
  - Ta with H_2O moderator
  - Be block (En > 1 MeV)
- Neutron production (Ta target)
  - 10^{11} neutrons/pulse
  - 10^{14} n/sec at 50 kW 5×10^{18} n/sec (peak)

ORELA Facility Details, cont.

- Neutron spectrum (Ta target)
  - 4 × 10^{13} n/MeV/sec at 1 MeV
  - 4 × 10^{10} n/MeV/sec at 14 MeV
- Number of
  - flight paths = 10
  - flight stations = 18
- Flight path lengths = 9 to 200 m
- For additional details, see the web site http://www.phy.ornl.gov/orela/orela.html/

CERN nTOF Facility details

- Proton energy ~80 GeV
  - 7 ×10^{12} protons / pulse (dedicated), ~50 % (parasitic)
- Neutron targets: natural Pb
- Neutron production
  - 10^6 neutrons in 0.14 eV to 150 MeV with 1 cm collimator
- Number of flight paths = 1
- Number of flight stations = 1
- Flight path length = 185 m

CERN nTOF Facility details, cont.

- Natural lead target is 60 cm × 80 cm × 80 cm with 20-cm square hole in back side (so effectively 40 × 80 × 80)
- Target is surrounded by 5 cm of water moderator
- “Beam reducers” trim neutron beam to 60 & 40 cm
- Two collimators reduce beam to ~9 cm and ~ 1 cm
  - 1 cm for capture; larger for fission
- Proton beam: Gaussian ~ 6 nsec with 2.4 seconds between pulses
- Supercycle is 7 cycles: nTOF gets all of some cycles (“dedicated”) and portions of some cycles (“parasitic”)

Types of Differential Data

- transmission
- total cross section
- elastic cross section
  - (angle-integrated or differential)
- fission
- inelastic
- capture
- absorption
- reaction
- eta
- self-indication
- combinations of the above

SAMMY can accommodate all of these. Other options can be added with relative ease.

Integral data can also be included in SAMMY analyses –

- Thermal cross section
- Average integral
- Maxwellian average
- K_1, K_{eff}
- westcott's g-factor
- a
- Resonance integral
- Reaction Rates
- NJOY's a
- NJOY's ?

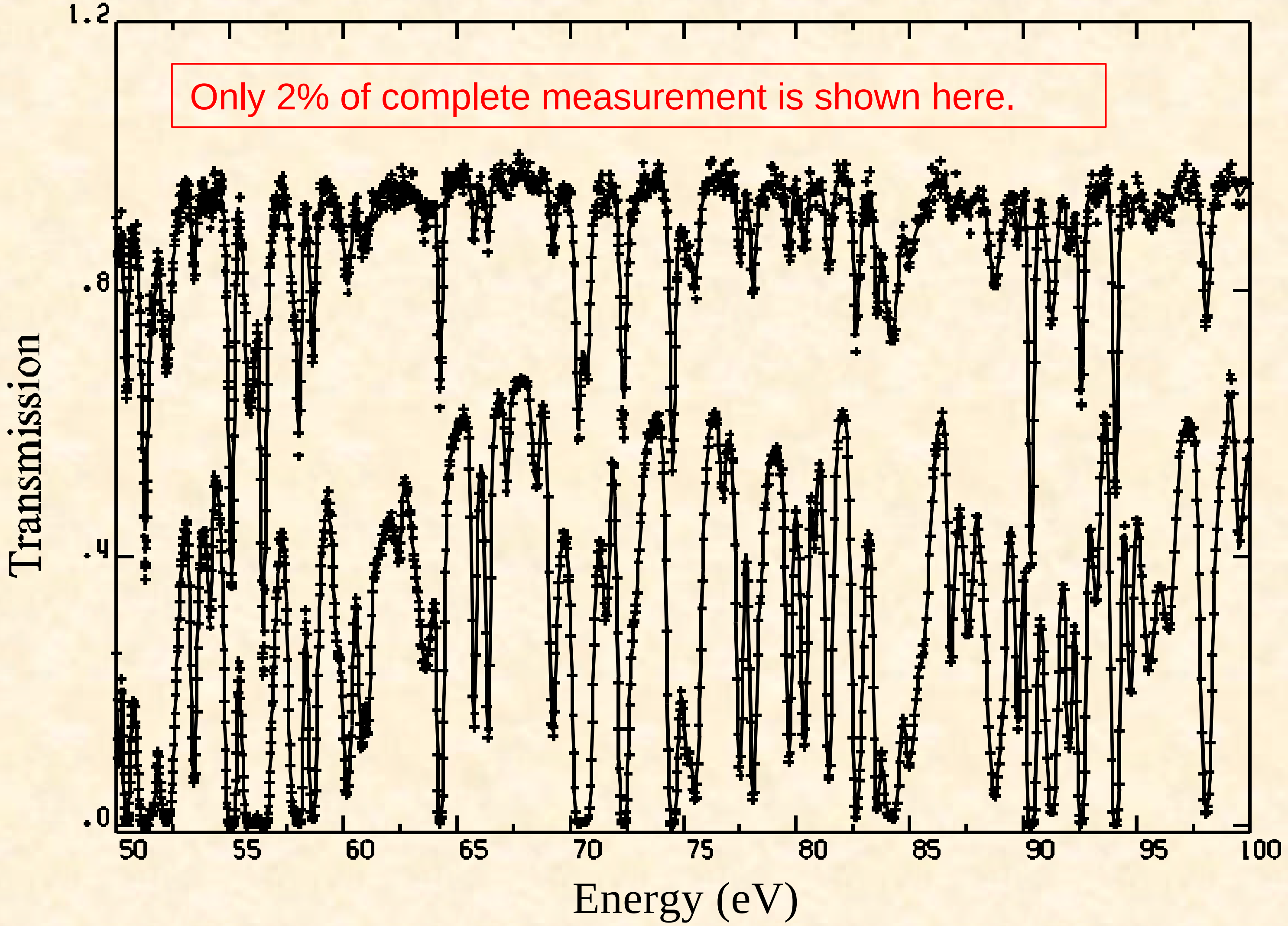
To be discussed later if time permits

Examples of differential data

1. Transmission example ^{235}U

- **^{235}U experimental and calculated neutron transmission in the energy range from 50 to 100 eV. Results of two sample thickness transmission experiments of Harvey et al. are displayed.**
  - **From the ORNL evaluation of L. C. Leal, H. Derrien, N.M. Larson, and R.Q. Wright, *R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV*, ORNL/TM-13516, Oak Ridge National Laboratory (November 1997). Also *Nucl. Sci. and Eng.* 131, 230 (February 1999).**

Transmission data example: ^{235}U

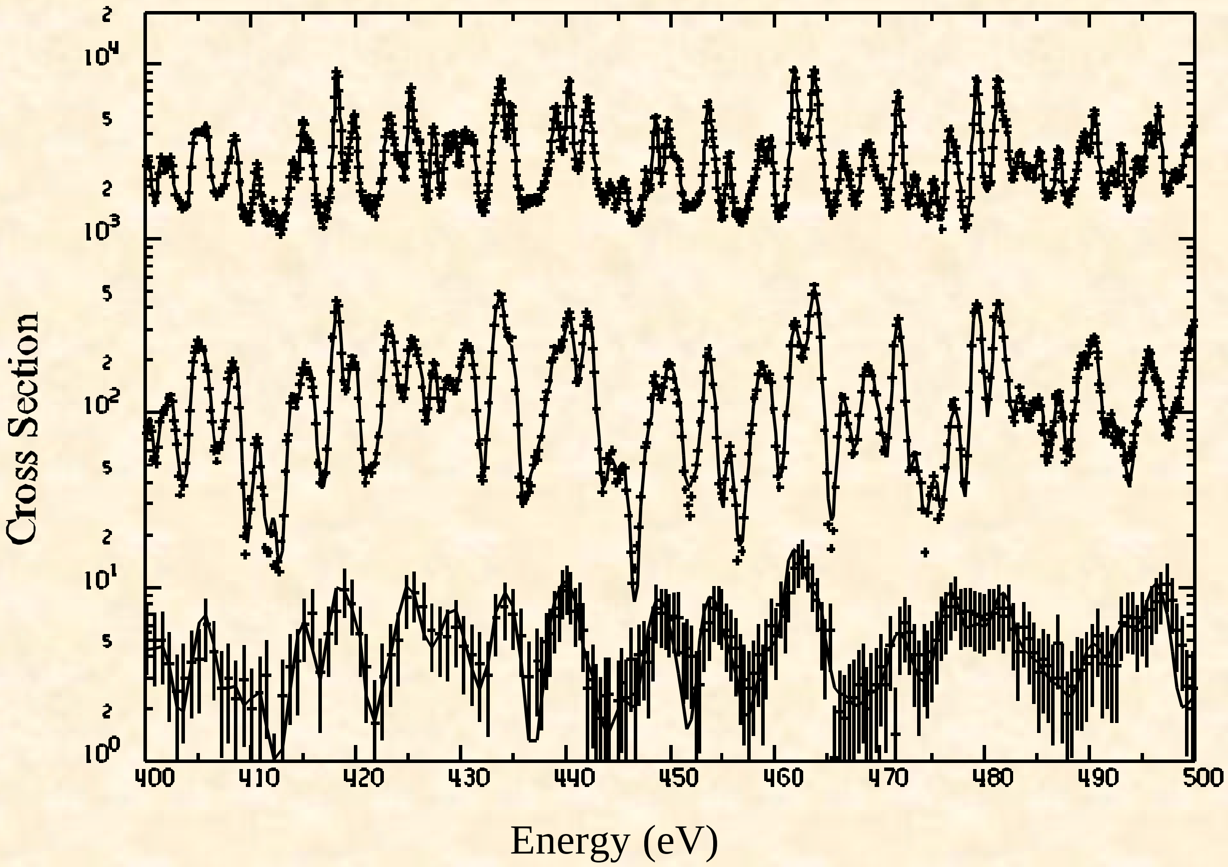


Only 2% of complete measurement is shown here.

thin

thick

2. Total, fission, & capture on ^{235}U



total
x100

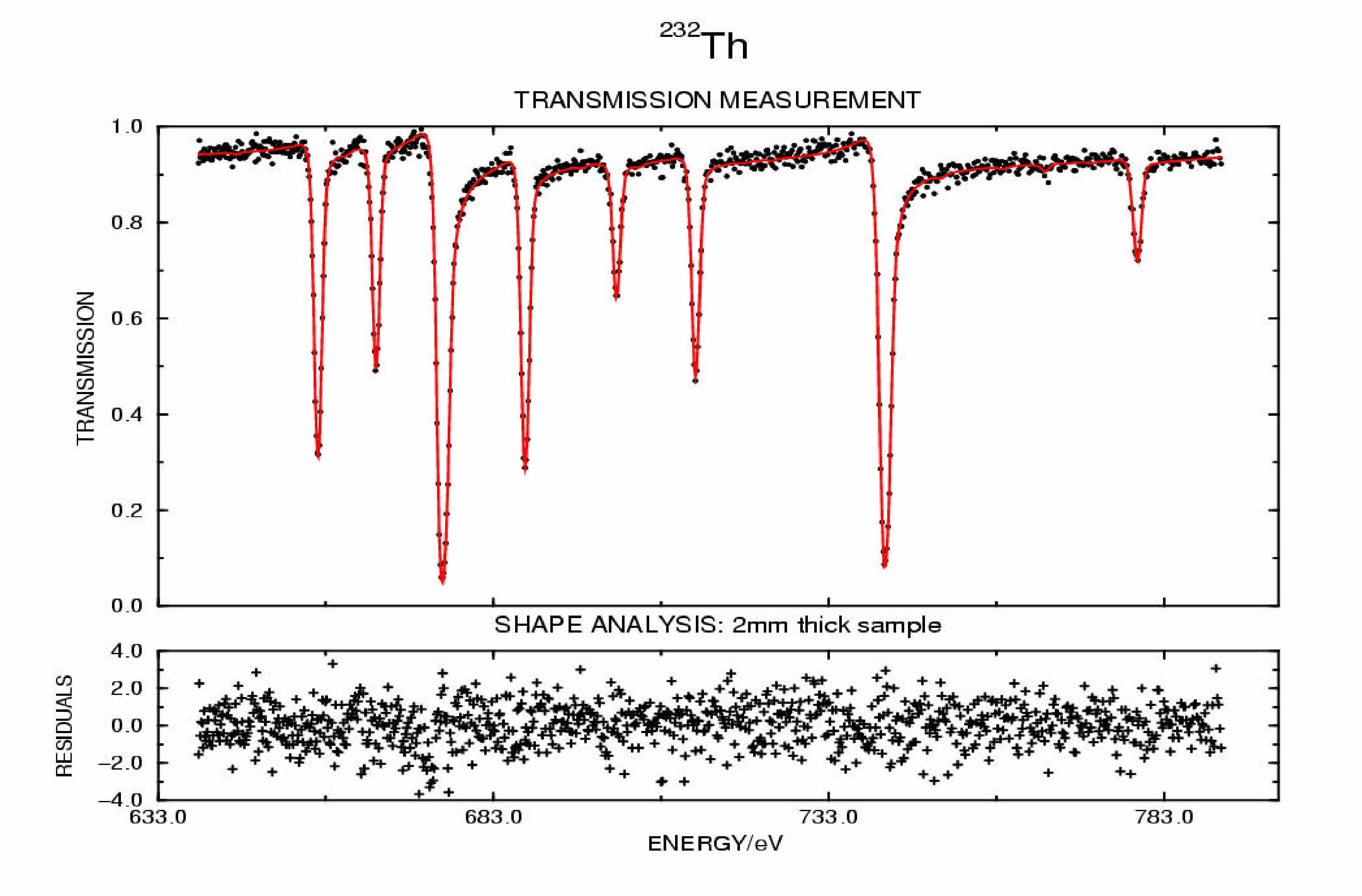
fission
x10

capture

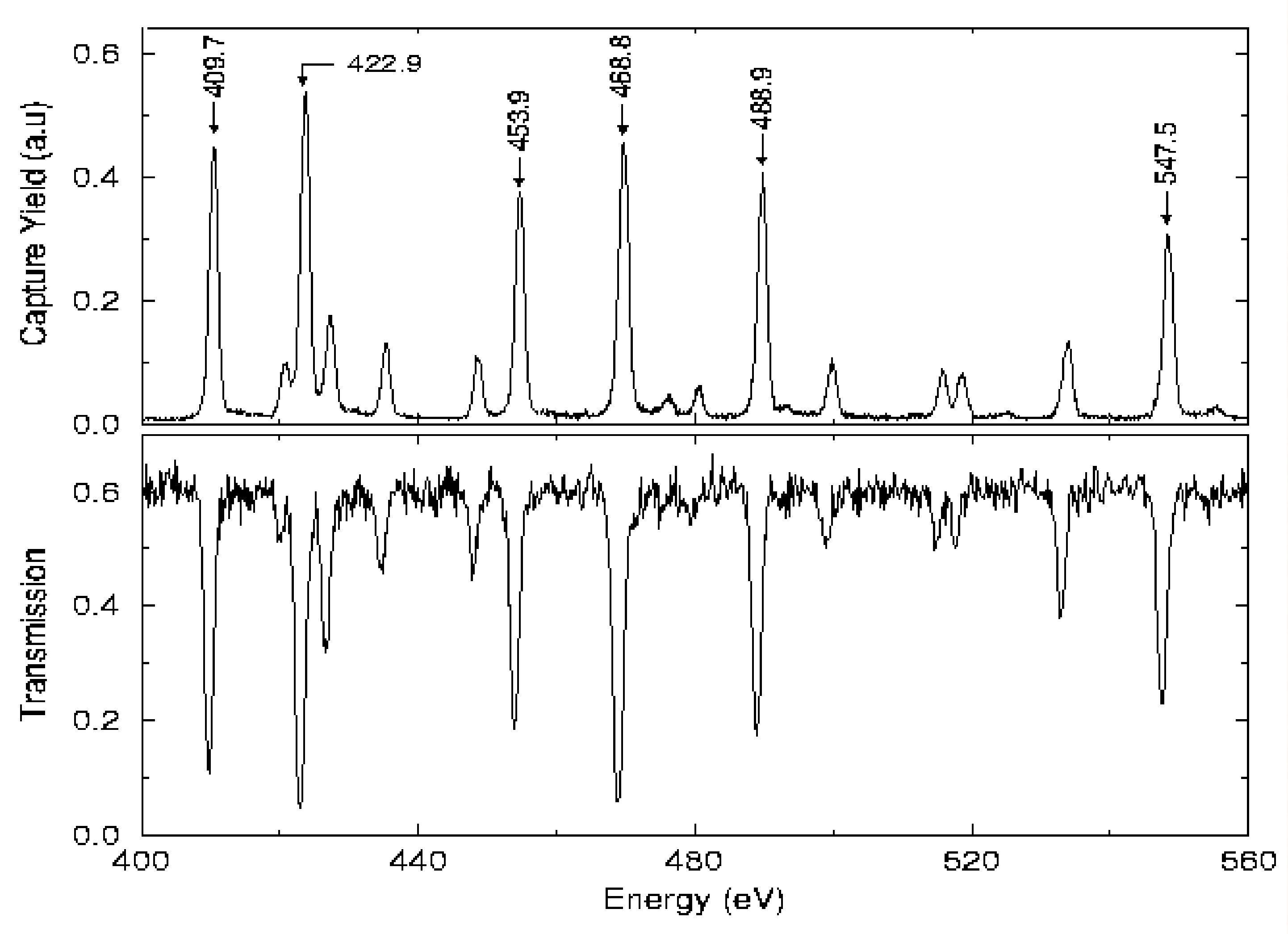
^{235}U experimental and calculated total cross section, fission cross section, and capture cross section in the energy range from 400 to 500 eV. Harvey et al. total cross section (multiplied by 100), Weston fission (multiplied by 10), and deSaussure capture cross sections are displayed.

3. ^{232}Th transmission

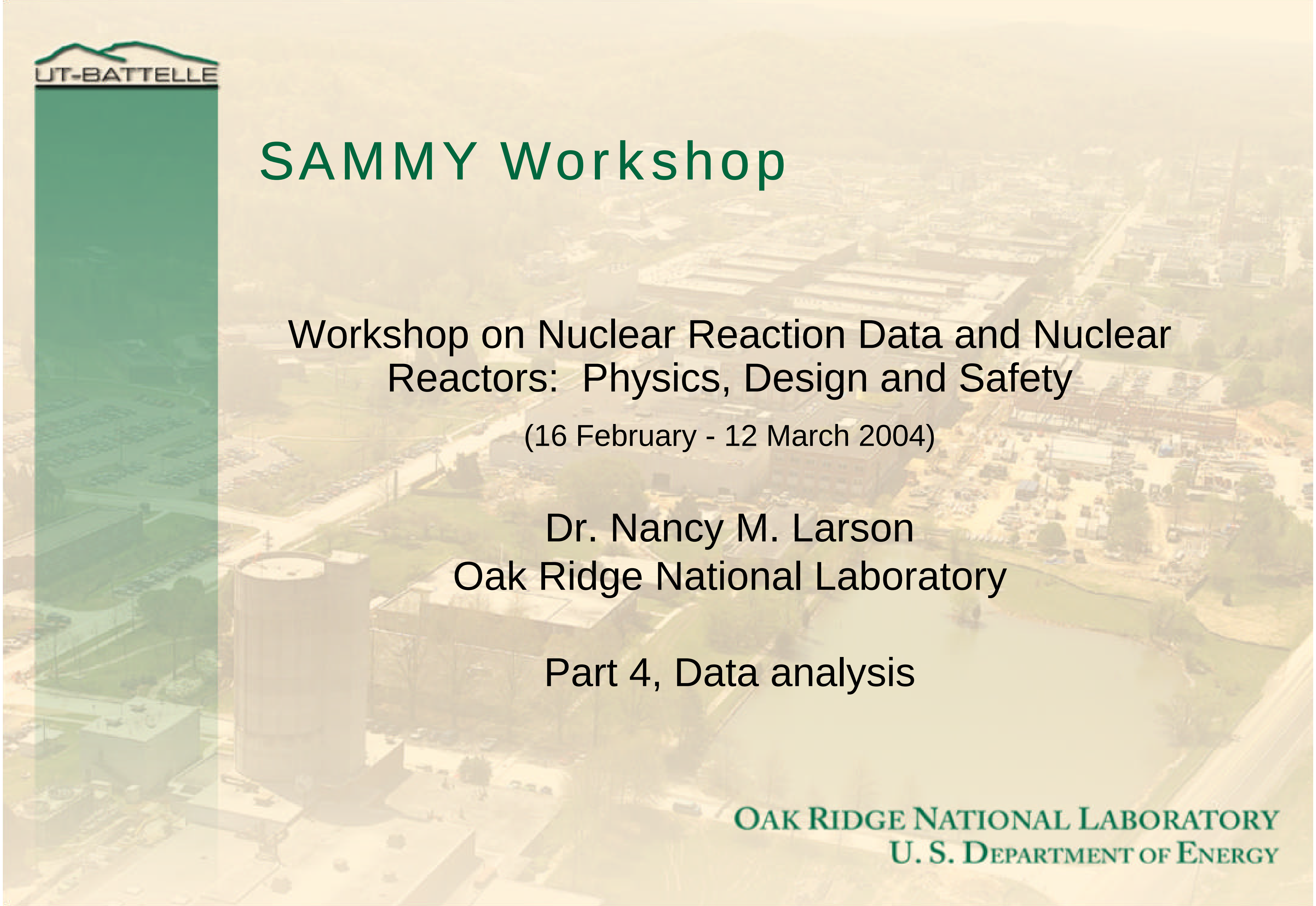
Plot courtesy of Peter Schillebeeckx, Geel



4. Capture and Transmission of ^{129}I



Plot courtesy of Peter Schillebeeckx of IRMM/Geel



SAMMY Workshop

Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety

(16 February - 12 March 2004)

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 4, Data analysis

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Three requirements

for analysis of neutron cross-section data in the resolved-resonance region

1. **Formalism for calculation of cross section**

Well understood – we've known how to do this since 1950's

2. **Mathematical description of experimental effects**

Impossible to do correctly! The best we can do is to make better-and-better approximations as time goes on.

3. **Fitting procedure, including treatment of covariances**

Reasonably well understood, but seldom done properly

Three requirements, cont.

- All three are included in SAMMY
  - Formalism
  - Experimental effect
  - Fitting procedure

- (SAMMY also includes many other features, not included in these “requirements”)

1. Formalism for calculation of cross sections

Scattering Theory

- Also called: Collision Theory or R-Matrix Theory

- Definitive Paper:
  - Lane & Thomas, "R-Matrix Theory of Nuclear Reactions", *Reviews of Modern Physics* **30**, 257-353 (1958)
- Easier-reading Book:
  - Foderaro, *The Elements of Neutron Interaction Theory*, The MIT Press, Cambridge MA and London, England (1971)

- (There are many other resources on this topic)

Other valuable references:

- **F. H. Fröhner, "Applied Theory of Resolved and Unresolved Resonances," *Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications*, M.K. Mehta and J.J. Schmidt (eds.), World Scientific, Singapore (1989)**
  - **Work was initially presented at ICTP Winter Courses on Nuclear Physics and Reactors, 1978.**
  - **A comprehensive and useful guide to applied neutron resonance theory**
  - **A variety of topics — preparation of data, the various approximations to R-matrix theory, Doppler broadening, experimental complications, data-fitting procedures, statistical tests**

- **F. H. Fröhner, "Theory of Neutron Resonance Cross Sections for Safety Applications," KFK 5073, Kernforschungszentrum Karlsruhe (1992)**
  - **Review paper prepared for the "Workshop on Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety," held at the ICTP, Trieste, Italy, 10 Feb. - 13 March 1992**
  - **Updated version of the first paper... covers many of the same topics**

- **F. H. Fröhner, "Evaluation and Analysis of Nuclear Resonance Data," JEFF 18 (2000)**
  - **From the forward to this report – "describes in detail two elements necessary to perform a correct analysis of experimental data in the resonance energy range: the neutron-nucleus interaction theory in this energy range and the mathematical formalism of statistical inference."**

Scattering Theory…

- **Is mathematically rigorous (but usually approximated)**
- **Describes what is actually measured but not what happens inside the nucleus**
  - **(i.e. the neutron-nucleus interaction is not explicitly included)**
- **Parameterizes in terms of**
  - **interaction radii & boundary conditions**
  - **resonance energies & widths**
  - **quantum numbers**

Why parameterize the cross sections? Why not just use the measured data?

(for more details, see Frohner's papers)

- **Too much information, too little understanding**
  - cross section vs energy ➔ ~100,000's of numbers
  - angular distributions have even more numbers
  - human minds seldom make sense of this many numbers!

- **Not enough information ➔ extrapolations are needed for practical applications**
  - other energies or energy regions
  - other experimental conditions:
    - temperature (Doppler broadening)
    - geometry (self-shielding calculations, multiple-scattering effects, etc.)
  - other nuclides (?)

Multilevel R-Matrix Theory

- **phenomenological**
  - describes what is seen (i.e. the measured cross sections)
  - does not describe what is not seen (i.e. the underlying nuclear physics)

- **mathematically correct**
  - analytic, unitary, rigorous

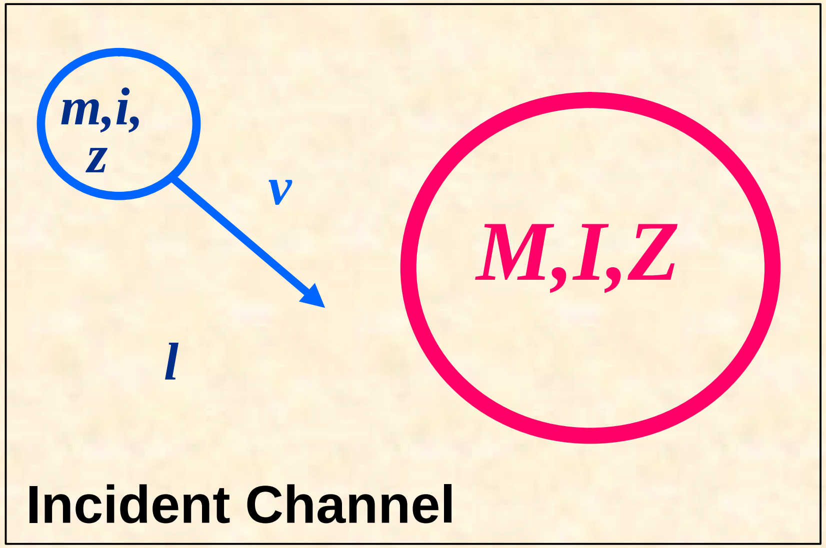
But is nearly always approximated in some fashion

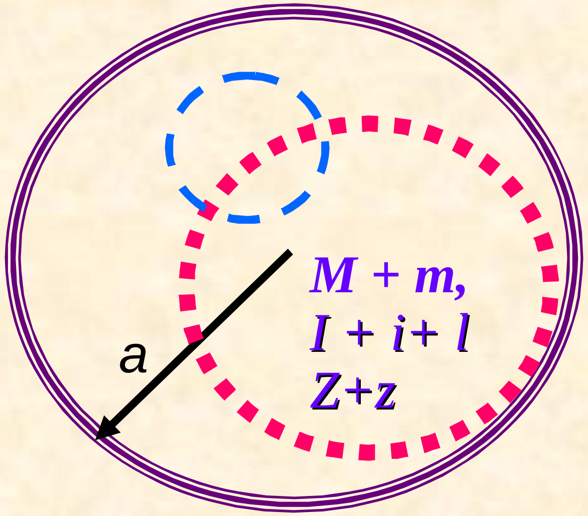
- **based on the following assumptions (re Lane & Thomas):**
  - The applicability of nonrelativistic quantum mechanics
  - The absence or unimportance of all processes in which more than two product nuclei are formed
  - The absence or unimportance of all processes of creation or destruction
  - The existence of a finite radial separation beyond which no nuclear interactions occur

Coulomb interaction is treated explicitly

Definitions of terms

- ***Channel***
  - **pair of (incoming or outgoing) particles**
  - **illustrated on next slide**

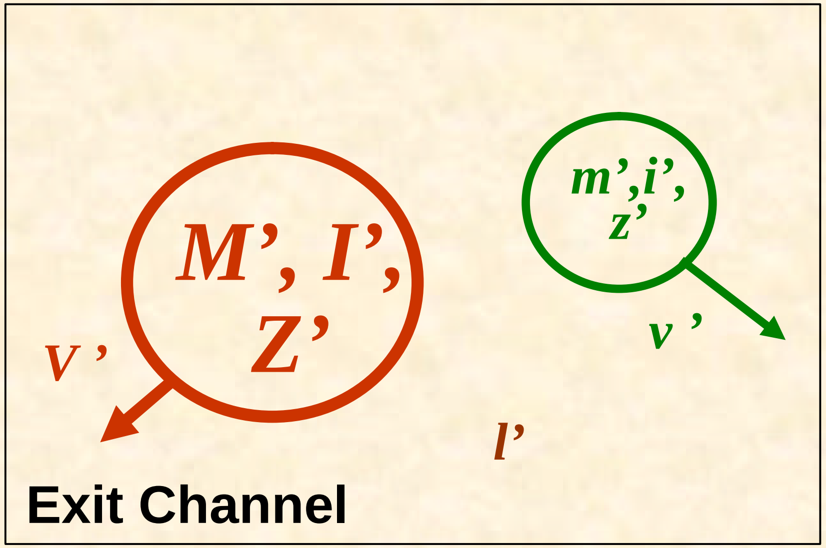




Outside *r* >*a* there is no interaction
(except Coulomb)

Inside *r* >*a* we do not know what happens

Some channels can be both incident and exit. Others are exit only (e.g., fission fragments).



Definitions of terms

- ***Channel***
  - **pair of (incoming or outgoing) particles, defined by *mass*, *charge*, and *spin quantum numbers***
- ***Mass***
  - **atomic mass of the particles**
  - **neutron mass = 1.008665 amu**
  - ***amu* = atomic mass unit, from Nuclear Wallet Cards:**

```
= 1.49241909 × 10-3 erg    = 7.51300563 × 1012 /cm
= 9.3149432 × 108 eV       = 1.0809478 × 1013 K
= 2.25234242 × 1023 / sec = 1.6605402 × 10-24 g
```

- ***Charge* = *Z* for nuclide, 0 for neutron, 1 for proton**
- **Spin quantum numbers (see next page)**

Definitions of terms, continued

- ***spin quantum numbers***
    - **(Note unprimed ➔ incident, primed ➔ exit):**

Each of these also has an associated parity.

- – **i = intrinsic spin of incident neutron = ½** **+1**
- – **I = spin of target nuclide = integer or ½ -integer** **p**
- – **l = relative orbital angular momentum (*s, p, d, f*, ...) (*l* = 0, 1, 2, 3,...)** **$(-1)^{l}$**
- – **s = channel spin** $\vec{s}=\vec{I}+\vec{i}$ **(+1) (p)**
- – **J = total spin for channel** $\vec{J}=\vec{s}+\vec{l}$ **$(+1)\ (p)\ (-1)^{l}$**

- **Required: conservation of spin and parity**
    - **(spin of incident channel = $J^{p} = J'^{p'}$ = spin of exit channel)**

Angular momentum addition rules

(for those unfamiliar with vector algebra)

If vector spin $\mathbf{a}$ is given by

$$\mathbf{a} = \mathbf{b} + \mathbf{c}$$

then a (the magnitude of $\mathbf{a}$) is within the limits

$$| b - c | = a = b + c$$

and a is either integer

(if b and c are both integer or both half-integer)

or half-integer

(if one of b and c is integer and the other half-integer)

Table shows angular momentum summations for 0, 1/2, 1, 3/2, and 2

b	*c*	*a = b + c*
0	0	0
0	1/2	1/2
0	1	1
0	3/2	3/2
0	2	2
1/2	1/2	0,1
1/2	1	1/2,3/2
1/2	3/2	1,2
1/2	2	3/2,5/2
1	1	0,1,2
1	3/2	1/2,3/2,5/2
1	2	1,2,3
3/2	3/2	0,1,2,3
3/2	2	1/2,3/2,5/2,7/2
2	2	0,1,2,3,4

Multilevel R-matrix theory

$$s^{total} = \frac{2p}{k^{2}} \sum_{J} g_{J} \sum_{\substack{incident \\ channels\ c}} \left(1 - \mathrm{Re}\left(U_{cc}^{J^{p}}\right)\right)$$

(There are similar equations for other cross section types)

Scattering matrix

$$U_{cc'}^{J} = \Omega_{l} W_{cc'}^{J} \Omega_{l'} \qquad \Omega_{l} = e^{-ij_{l}}$$

$$W = P^{1/2}\left(I - RL\right)^{-1}\left(I - RL^{*}\right)P^{-1/2} \qquad L = \left(S - B\right) + iP$$

R-matrix

$$R_{cc'} = \sum_{l} \frac{g_{lc} g_{lc'}}{E_{l} - E - i\Gamma_{l}^{g}} \qquad \Gamma_{lc} = 2P_{l}\left(g_{lc}\right)^{2}$$

Resonance parameters (values are needed in R-matrix codes)

Multilevel R-matrix theory, continued

$$R_{cc'} = \sum_{l} \frac{g_{lc} g_{lc'}}{E_l - E - i\Gamma_l^g}$$

The presence of capture width in denominator is what makes Reich-Moore different from "full" R-matrix.

Multilevel R-matrix theory, continued

- **Complete list of definitions, equations, derivations, etc., are available**
  - **in the SAMMY users' manual**
  - **in extended lecture notes**
    - **We will cover this during the lectures only if time permits**
    - **Ask for handout …**

File 4x1.pdf