Theory for low-energy nuclear reactions

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Lawrence Livermore National Laboratory

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Outline

- Why are we interested in low-energy reactions?
 Why do we need theory to describe reaction processes?
- What types of reactions are relevant in this context?
- How do we describe compound-nuclear reactions?
- Which physics models and inputs are needed?
- Challenges and open questions

Why are we interested in low-energy reactions?

Why do we need theory to describe reaction processes?



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Goals of advanced reaction theory

- Achieve deeper understanding of underlying microscopic processes in reaction experiments
- Determine of degrees of freedom relevant to the interaction between projectile and target

Determine cross sections needed for applications

- Astrophysics
- Nuclear energy
- National security



Extract nuclear structure information from reaction experiments

- Inform and test nuclear structure theories
- Determination of nuclear structure inputs for calculations



Low-energy reactions remain essential



- Stable beams & targets
- Probes of nuclear structure in/near valley of stability
- Nuclear radii, density distributions, levels, spins & parities, shell gaps, spin-orbit, tensor force, 2-nucleon correlations
- Direct measurements of cross sections
- Exotic beams on stable targets
 - Study structure outside the valley (r-process, fission fragments, etc.)
 - Pushing theory to new limits
 - Indirect measurements of cross sections using RIBs





What types of reactions are relevant in this context?

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Describing low-energy reactions

Basic notation

- Reaction: a + A -> c + C + Q
- Alternative: A(a,c)C
- a + A : projectile and target (entrance channel)
- c + C : electile and residual nucleus (exit channel)
- Q-value: $Q = E_f E_i$

Q>0 : exothermic (releases energy) Q<0 : endothermic (requires energy)

- Partition: combination of particles
- Channel: specified by partition plus state of excitation of nuclei

Closed: not accessible for given E Open: energetically accessible

Observable: cross section

- Measured or calculated
- Definition:

 $\sigma =$

particles c emitted

- (#particles a incident/unit area) (#target nuclei)
- Units: 1 barn = 10^{-28} m^2

Classification

- By observed entrance-exit channel combination
- By number of degrees of freedom excited (related to time scales)

'Low energy' reactions

- Involve collective, single-nucleon, few nucleon excitations
- Exit channel contains 2 (or three) fragments

Classification

by observed entrance-exit channel combination

Two particles in exit channel

- Elastic scattering: A(a,a)A
 Internal states unchanged
 ²⁰⁸Pb(n,n)²⁰⁸Pb
- Inelastic scattering: A(a,a)A*

Target and/or projectile excited ${}^{90}\text{Zr}(\alpha,\alpha'){}^{90}\text{Zr}^{*}$

• Transfer reaction: A(a,c)C

Stripping: transfer part of projectile to target ⁹⁰Zr(d,p)⁹¹Zr*

Pickup: transfer part of target to projectile 157 Gd(3 He, α) 156 Gd*

• Charge exchange: A(a,c)C

Mass numbers remain the same ${\rm ^{14}C(p,n)^{14}N}$

More classes....

- Capture: A(a,γ)C
 Projectile is captured, energy radiated
 ⁷Be(p,γ)⁸B, ¹³⁰Sn(p,γ)¹³¹Sn
- Breakup:

Projectile breaks apart in target field d+⁹⁰Zr -> ⁹⁰Zr*+p+n

• Knockout:

Nucleon/light nucleus emitted from target, projectile continues on Example: A(e,e'p)B

Combinations of these processes can occur in a reaction.

Classification by degrees of freedom excited

Direct reactions

- few collisions, fast: 10⁻²¹-10⁻²²s
- target structure largely intact
- forward-peaked
- involve single-particle excitations

Compound reactions

- multiple collisions, slow: 10⁻¹⁵-10⁻¹⁶s
- target fuses with projectile
- symmetric wrt 90° axis
- involve many-particle excitations



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Typical angular distributions for direct and CN reactions. **Angular distributions**



Classification by degrees of freedom excited

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Single-particle vs. many-particle excitations



Now: Focus on Compound Reactions





How do we describe compoundnuclear reactions?





Resonances, from isolated to strongly overlapping



Nuclear Reactions (1980)

Resonances, from isolated to strongly overlapping



Evaluated (n, γ) cross sections from thermal to 20 MeV (ENDF/B-VII)

The demarcation between the resolved and unresolved resonance regions, and the Hauser-Feshbach regime, depends on mass region and proximity to closed shells.

Hauser-Feshbach formalism: A hint of a derivation

Ingredients

• Bohr's hypothesis: formation and decay of CN are independent

 $\sigma_{\alpha\chi}(\mathsf{E},\mathsf{J},\pi) = \sigma_{\alpha}^{\mathsf{CN}}(\mathsf{E},\mathsf{J},\pi) \cdot \mathsf{G}_{\chi}^{\mathsf{CN}}(\mathsf{E}^{\mathsf{CN}},\mathsf{J},\pi)$

• Principle of detailed balance: time-reverals invariance of reaction

 $\mathbf{k}_{\alpha}^{2}\sigma_{\alpha\chi}=\mathbf{k}_{\chi}^{2}\sigma_{\chi\alpha}$

• Combining this, one obtains the partial CN cross section

 $\sigma_{\alpha\chi}(\mathsf{E},\mathsf{J},\pi) = \mathsf{k}_{\alpha}^{2} \sigma_{\alpha}^{\mathsf{CN}}(\mathsf{E}_{\alpha},\mathsf{J},\pi) \sigma_{\chi}^{\mathsf{CN}}(\mathsf{E}_{\chi},\mathsf{J},\pi) / \Sigma_{\chi'} \mathsf{k}_{\chi'}^{2} \sigma_{\chi'}^{\mathsf{CN}}(\mathsf{E}_{\chi'},\mathsf{J},\pi)$

• Introducing transmission coefficients

 $\sigma_{\alpha}^{\text{CN}}(\mathsf{E}_{\alpha},\mathsf{J},\pi) = \pi \ \mathsf{k}^{-2}{}_{\alpha} \ (2\mathsf{J}+1) \ \mathsf{T}_{\alpha}^{-\mathsf{J}}$

• We obtain the CN cross section (for fixed J,π)

$$\sigma_{\alpha\chi}(\mathsf{E},\mathsf{J},\pi) = (\mathsf{2J+1}) \frac{\pi \ \mathsf{T}_{\alpha}^{\mathsf{J}} \mathsf{T}_{\chi}^{\mathsf{J}}}{\mathsf{k}^{2}_{\alpha} \ \Sigma_{\chi}^{\mathsf{J}} \mathsf{T}_{\chi}^{\mathsf{J}}}$$

Hauser-Feshbach calculations: physics input



Quantities required

- Transmission coefficients T_{χ} for all channels χ : neutron, proton, charged particles, γ , fission
- Level densities for nuclei involved
- Discrete levels with J,π

HF calculations for compound-nucleus cross sections

Average cross section per unit energy in the outgoing channel: $\frac{d\sigma_{\alpha\chi}^{HF}}{dE_{\chi}} = \pi \lambda_{\alpha}^2 \sum_{J\Pi} \omega_{\alpha}^J \sum_{lsl'sl'} \frac{T_{\alpha ls}^J T_{xl's'}^J \rho_{l'}(U)}{\sum_{x^n l^n s^n} T_{x^n l^n s^n}^J + \sum_{x^n l^n s^n} \int T_{x^n l^n s^n}^J (E_{\chi^n}) \rho_{l''}(U'') dE_{\chi^n}}$ Evaluating this expression requires knowledge of optical potentials and the structure of the nuclei that can be reached in the decay of the CN: (n,3n) (n,γ) (n,n') (n,2n)Neg. parity A-1X Pos. parity Isomer W.E. Ormand (LLNL)

Finding a code...

Hauser-Feshbach codes:

- Many Hauser-Feshbach codes have been written: STAPRE, TALYS, EMPIRE, MCNASH, COH, SMOKER, NON-SMOKER, YAHFC,....
- Publicly available, widely used, documented, and supported: TALYS and EMPIRE





Talys:

- Developers: A. Koning, S. Hilaire, M. Duijwestijn (NRG Petten, Netherlands, and CEA Bruyere-le-Chatel, France)
- Website: www.talys.eu/home/
- Reference: Koning & Rochman, NDS 113 (2012) 2841-2934
- Interesting feature: minimal input file requires only 4 pieces of information: Proj, Z_T, A_T, E

Empire:

- Developers: M. Herman et al. (BNL, IAEA, Bucharest, Lubljana, LLNL, Brazil, Bratislava, KAERI, Kiev)
- Website: www.nndc.bnl.gov/empire/index.html
- Reference: Herman et al, NDS 108 (2007) 2655-2715
- Interesting feature: code versions named after battles fought by Napoleon Bonaparte

Getting the physics inputs...

Good starting points:

- Use default models and parametriziations, read the manuals for instructions on improvements
- Consult RIPL "Reference Input Parameter Library": web site and review paper
 www-nds.iaea.org/RIPL-3



Lest Updated: 07/16/2013 07:20:4



Available online at www.sciencedirect.com

ScienceDirect

Nuclear Data Sheets

Nuclear Data Sheets 110 (2009) 3107-3214



RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

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 Bhabba Atomic Research Center, Trombus, 400088 Mumbat, India 14 JUKO Research, NL-1817 Alkmaar, The Netherlands ¹⁵ Joint Institute for Power and Nuclear Research – Sosny, BY-220109 Minsk, Belarus Retired in 1998, Ente Nuove Tecnologie, Energia e Ambiente (ENEA), 40129 Bologna, Italy and ¹⁷ Nuclear Physics Department, Bucharest University, 077125 Bucharest-Maquele, Romania

(Received July 20, 2009)

We describe the physics and data included in the Reference Input Parameter Library, which is devoted to input parameters needed in calculations of nuclear reactions and nuclear data evaluations. Advanced modelling codes require substantial numerical input, therefore the International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of validated nuclear-model input parameters, referred to as the Reference Input Parameter Library (RIPL). A final RIPL coordinated research project (RIPL-3) was brought to a successful conclusion in December 2008, after 15 years of challenging work carried out through three consecutive IAEA projects. The RIPL-3 library was released in January 2009, and is available on the Web through http://www.nds.teac.org/RIPL-3/. This work and the resulting database are extremely important to theoreticians involved in the development and use of nuclear reaction modelling (ALCE, EMPIRE, GNASH, UNF, TALYS) both for theoretical research and nuclear data evaluations.

The numerical data and computer codes included in RIPL-3 are arranged in seven segments: MASSES contains ground-state properties of nuclei for about 9000 nuclei, including three theoretical predictions of masses and the evaluated experimental masses of Audi et al. (2003). DISCRETE LEVELS contains 117 datasets (one for each element) with all known level schemes, electromagnetic and γ-ray decay probabilities available from ENSDF in October 2007. NEUTRON RESONANCES contains average resonance parameters prepared on the basis of the evaluation performed by Ignatyuk and Maghabghab. OPTICAL MODEL contains 495 sets of phenomemological optical model parameters defined in a wide energy range. When there are insufficient experimental data, the evaluator has to resort to either global parameterizations or microscopic approaches. Radial density distributions to be used as input for microscopic calculations are stored in the MASSES segment. LEVELD DENSITIES contains phenomemological parameters dualities in eiroscopic single-particle level scheme. Partial level densities formulae are also recommended. All tabulated total level densities are consistent with both the resonances, experimental gamma-ray strength functions and mothods for calculating parmate parameters that quantify giant resonances, manneters and discrete levels. GAMMA contains parameters that quantify giant resonances, corporimental GDR parameters are represented by Lorentian fits to the photo-absorption cross sections for 102 nuclides ranging from ⁵¹V to ²²⁰Pp. FISSION includes global prescriptions for fission barriers and nuclear level densities are fission sadfile points based on microscopic HPB calculations constrained by experimental data reso densities.

*) Corresponding author, electronic address: r.eapotenoy@iaea.org; roberto.capote@yahoo.com

Capote *et al*, Nuclear Data Sheets 110 (2009) 3107 23 authors, 108 pages, many years...

Checking the calculations...

Experimental data and evaluations:

- National Nuclear Data Center: www.nndc.bnl.gov
- CSISRS (EXFOR): Nuclear reaction experimental data
- ENDF (and other evaluations): Evaluated Nuclear (reaction) Data File
- NuDat: Nuclear structure and decay Data
- And many more resources: Codes, publications, meeting info, …





Points to remember:

- Nuclear physics input is provided through data bases or by the user
- Models and input parameters are not unique, calculating a good cross section is both art *and* science
- The old principle holds: garbage in → garbage out
- Make use of cross-checks, whenever possible

Which physics models and inputs are needed?





Optical model potentials

Optical model potential

- Reduces complicated interaction of projectile with target to effective one-body problem
- Imaginary components account for channels not explicitly treated (loss of flux)
- Formally, a complicated function (non-local, energy dependent)
- Practical applications use
 phenomenological forms
- Popular: Woods-Saxon shape

 $\mathcal{U}(r, E) = -\mathcal{V}_V(r, E) - i\mathcal{W}_V(r, E) - i\mathcal{W}_D(r, E)$ $+ \mathcal{V}_{SO}(r, E).\mathbf{I}.\sigma + i\mathcal{W}_{SO}(r, E).\mathbf{I}.\sigma + \mathcal{V}_C(r),$

$$\mathcal{V}_{V}(r, E) = V_{V}(E)f(r, R_{V}, a_{V}),$$

$$\mathcal{W}_{V}(r, E) = W_{V}(E)f(r, R_{V}, a_{V}),$$

$$\mathcal{W}_{D}(r, E) = -4a_{D}W_{D}(E)\frac{d}{dr}f(r, R_{D}, a_{D}),$$

$$\mathcal{V}_{SO}(r, E) = V_{SO}(E)\left(\frac{\hbar}{m_{\pi}c}\right)^{2}\frac{1}{r}\frac{d}{dr}f(r, R_{SO}, a_{SO}),$$

$$\mathcal{W}_{SO}(r, E) = W_{SO}(E)\left(\frac{\hbar}{m_{\pi}c}\right)^{2}\frac{1}{r}\frac{d}{dr}f(r, R_{SO}, a_{SO}).$$

►
$$f(r, R_i, a_i) = (1 + \exp[(r - R_i)/a_i])^{-1}$$
,

Nucleon-nucleus OMP Koning & Delaroche, NPA 713 (2003) 231



Hauser-Feshbach calculations: Discrete states and level densities

Level densities above E_{cut}

- Cover energy regime above highest included discrete level
- Microscopic and phenomenological models available
- Reproduce related measurements, e.g. resonance spacing at S_n
- Parametrizations of popular models, and tables of microscopic LDs available at RIPL-3 web site

Discrete states below E_{cut}

- Complete E,J, π information
- Branching ratios for γ-decay
- ENSDF & NuDat databases at NNDC
- Reproduced at RIPL-3 website



From: R.B. Firestone

Hauser-Feshbach calculations: γ-ray transmission coefficients

γ-ray strength function

- Gives TC: $T^{\gamma}_{XL}(\epsilon) = 2\pi \epsilon^{2L+1} f^{\gamma}_{XL}(\epsilon)$
- E1 dominates
- Various phenomenological forms exist, mostly variants of Lorentzian
- RIPL-3 gives GDR parameters $\mathsf{E}_{\mathsf{GDR}},\!\Gamma,\!\sigma$
- Constraint radiative width:

$$\overleftarrow{f}_{\mathrm{XL}}(\epsilon_{\gamma}) = \epsilon_{\gamma}^{-(2L+1)} \frac{\langle \Gamma_{\mathrm{XL}}(\epsilon_{\gamma}) \rangle}{D_{l}}$$

• Related to photo-absorption xsec:

$$\vec{f}_{\rm EL}(\epsilon_{\gamma}) = \frac{\epsilon_{\gamma}^{-2L+1}}{(\pi\hbar c)^2} \frac{\langle \sigma_{\rm XL}(\epsilon_{\gamma}) \rangle}{2L+1}$$

Microscopic theories predict γSF



Daoutidis & Goriely, PRC 86 (2012) 034328

Hauser-Feshbach calculations: Level density prescriptions

Gilbert-Cameron

• Product form:

$$\rho(E_x, J, \pi) = P(E_x, J, \pi) R(E_x, J) \rho^{tot}(E_x)$$

$$R(E_x, J) = \frac{2J+1}{2\sigma^2} \exp\left[-\frac{(J+1/2)^2}{2\sigma^2}\right]$$

- Back-shifted Fermi-Gas at high E: $\rho_F^{\text{tot}}(E) = \frac{1}{\sqrt{2\pi}\sigma} \frac{\sqrt{\pi}}{12} \frac{\exp\left[2\sqrt{aU}\right]}{a^{1/4}U^{5/4}}$
- Constant-T at low E: $\rho_{CT}^{tot}(E_x) = \frac{dN(E_x)}{dE_x} = \frac{1}{T} \exp\left[\frac{E_x - E_0}{T}\right]$
- Constraints: cumulative number of levels at low E, resonance spacing at S_n



Alternatives

- Other phenomenological forms
- Theoretical predictions (SMMC, etc.)

CNR*2007 talk

Hauser-Feshbach calculations: fission model

Phenomenological Model

- Static, one-dimensional fission barriers along the deformation path, to be traversed
- Allows for calculation of T_{fiss}
- Single, double, or triple-humped fission barrier models
- Parameters: Heights, curvature hω, quasistationary states, transition states, level densities
- Parameters found in RIPL-3

Alternatives

- Microscopic calculations of fission barriers and level densities exist
- Truly dynamic descriptions of fission process is challenging



Beyond Hauser-Feshbach: Pre-equilibrium processes

Pre-equilibrium reactions

2.5 -

2.0

1.5

1.0 -

0.5

0.0 n (b)

Fission cross section (barns)

- Important contributions
- Models: Exciton, FKK, NWY, TUL
- Models incorporated in most codes (Talys, Empire)

Solid: with preequilibrium

Dashed: no preequilibrium

2nd chance

10

total

1st chance

5



Concluding remarks



Questions addressed today

- Why are we interested in low-energy reactions?
 Why do we need theory to describe reaction processes?
- What types of reactions are relevant in this context?
- How do we describe compound-nuclear reactions?
- Which physics models and inputs are needed?
- Challenges and open questions
- Many thanks to my collaborators....

Challenges and Open Questions

Improvements to physics inputs

- Optical models
- Level densities
- γ-ray strength functions
- Fission model

Reaction mechanisms

- Interplay of direct and compound reactions (preequilibrium)
- Modification of formalism for low level densities

Experiments

- Measurements of inputs (level densities, strength functions)
- Constraints for cross sections

Thanks to my Collaborators

Surrogate Reactions

<u>Theory</u>

Frank Dietrich, Daniel Gogny, Ian Thompson, Walid Younes (LLNL)

Experiment

- J. Burke, R. Casperson, R. Hughes, J.J. Ressler, N.D. Scielzo (LLNL) C. Beausang, T. Ross (U Richmond)
- J. Cizewski et al (Rutgers)



B. Sleaford and N.Summers (LLNL)R.B. Firestone, A. Hurst, S.Basunia (LBNL)

Reaction Theory.org

TORUS: Theory of Reactions for Unstable iSotopes A Topical Collaboration for Nuclear Theory

www.reactiontheory.org



TORUS members

Ian Thompson, LLNL Jutta Escher, LLNL Filomena Nunes, MSU Neelam Upadhyay MSU A. Mukhamedzhanov, TAMU L. Hlophe, OU V. Eremenko, OU Charlotte Elster, OU Goran Arbanas, ORNL





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• Related to photo-absorption xsec:

$$\vec{f}_{\rm EL}(\epsilon_{\gamma}) = \frac{\epsilon_{\gamma}^{-2L+1}}{(\pi\hbar c)^2} \frac{\langle \sigma_{\rm XL}(\epsilon_{\gamma}) \rangle}{2L+1}$$

- Microscopic theories predict γSF

$$\begin{aligned} \frac{f_{E1}(S_n)}{f_{M1}(S_n)} &= 0.0588 \cdot A^{0.878} \\ f_{E2}^{\gamma}(\epsilon) &= 7.2 \times 10^{-7} A_C^{2/3} f_{E1}^{\gamma}(S_n) \\ f_{M2}^{\gamma}(\epsilon) &= 2.2 \times 10^{-7} f_{E1}^{\gamma}(S_n) \\ f_{E3}^{\gamma}(\epsilon) &= 3.4 \times 10^{-13} A_C^{4/3} f_{E1}^{\gamma}(S_n) \\ f_{M3}^{\gamma}(\epsilon) &= 1.1 \times 10^{-13} A_C^{2/3} f_{E1}^{\gamma}(S_n) \end{aligned}$$



Benouaret, PRC 79 (2009) 014303

Reaction mechanisms in neutron capture

Capture contributions

Direct: single-step EM transition Semidirect: via GDR excitation Compound: via equilibrated CN

Relevance

What happens away from stability, where level densities are low?



Our work

- Implementation of DSD calculations
- Study of relative contributions
- Extension to include CN contributions



Thompson, Escher, Arbanas, ND2013 proceedings, submitted.

Challenge: cross sections for compound reactions



Surrogate Idea



J. Escher et al, Review of Modern Physics (2012)

Example: radiative capture



The Weisskopf-Ewing (WE) limit



Predicting compound-nuclear spin-parity distributions

Formation of a highly excited nucleus in a direct reaction

- inelastic scattering, pickup, stripping reactions
- various projectile-target combinations

Damping of the excited states into a compound nucleus

- competition between CN formation and non-equilibrium decay (particle escape)
- dependence on J^{π}



Satchler, Introduction to Nuclear Reactions (1980)



