Theoretical description of low-energy Coulomb excitation

Magda Zielińska IRFU/DPhN, CEA Saclay

- Why Coulomb excitation?
- Basic introduction to Coulomb-excitation theory
- Approximations and limitations

Low-Energy Coulomb Excitation and Nuclear Deformation, chapter in: *The Euroschool on Exotic Beams - Vol.6*, Lecture Notes in Physics 1005, 43 (2022).

Coulomb excitation: what's so great about it?

population of excited states via purely electromagnetic interaction between the collision partners



- B(E2) and B(E3) transition probabilities measure of collectivity
- direct measurement of quadrupole moments including sign ideal tool to study shape coexistence
- easy way to access non-yrast states and study their properties
- renaissance of the technique as ideally suited for state-of-the-art RIB facilities:
 - beam energies available perfect for Coulomb excitation (2-5 MeV/A)
 - high cross sections (excitation of 2⁺₁: barns)
 - practical at the neutron-rich side

Basic facts about Coulomb excitation

• Due to the purely electromagnetic interaction the nucleus undergoes a transition from state $|i\rangle$ to $|f\rangle$.

- Then it decays to the lower state, emitting a γ -ray (or a conversion electron).
- The matrix elements $\langle f||E2||i\rangle$ describe the excitation and decay pattern \rightarrow they are directly related to γ -ray intensities observed in the experiment.
- They are related to the nuclear shape and collectivity.

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• They are related to the nuclear shape and collectivity.

 \rightarrow from extensive sets of E2 matrix elements quadrupole invariants can be formed in order to deduce deformation parameters for individual states defined in the intrinsic frame of the nucleus.

Safe energy

• Cline's "safe energy" criterion: purely electromagnetic interaction if the distance between nuclear surfaces is greater than 5 fm

$$D_{min} = 1.25 \cdot (A_p^{1/3} + A_t^{1/3}) + 5.0$$
 [fm]

- empirical criterion based on systematic studies of inelastic and transfer cross-sections at beam energies of few MeV/A *W.J. Kernan et al. / Transfer reactions*
- other criteria established for high-energy Coulomb excitation
- one-neutron sub-barrier transfer recently observed in Coulomb excitation of ⁴²Ca on ²⁰⁸Pb (K. Hadyńska-Klęk et al, PRC 97, 024326 (2018).)



"Safe energy" requirement

...is due to the fact that D_{min} has to be sufficiently large. But it's not the only way to ensure it!



$$E(\theta_{CM}) = 0.72 \frac{Z_P Z_T}{D_{min}} \cdot \frac{A_P + A_T}{A_T} \left(1 + \frac{1}{\sin\left(\frac{\theta_{CM}}{2}\right)} \right) \qquad [MeV]$$

Two possibilities to prepare an experiment:

- choose adequate beam energy (D > D_{min} for all θ) low-energy Coulomb excitation
- limit scattering angle, i.e. select impact parameter b (E_b, θ) > D_{min} high-energy Coulomb excitation

Dependence of cross sections on energy



⁷⁴7n on ²⁰⁸Pb

⁴⁰S on ¹⁹⁷Au

- low-energy Coulomb excitation: maximum cross section for single- and multi-step excitation at \sim 4-5 MeV/A
 - stronger dependence of multi-step excitation cross sections on energy
- only single-step excitation important for energies of tens or hundreds MeV/A; slow decrease of cross section with energy
 - possibility to use very thick targets (g/cm²) to compensate for that

What else the cross sections depend on?

- strength of the electromagnetic field: atomic number of the collision partner
- beam energy
- difference in excitation energy between the initial and final levels
- scattering angle
- transition probabilities
- transition multipolarities
 - E2 excitation dominates, followed by E3; other multipolarities (including magnetic transitions) usually negligible in low-energy Coulomb-excitation process



Beyond the first perturbation

- Electromagnetic interaction well-known → one can easily calculate Coulomb-excitation cross section for any states of the investigated nucleus when its internal structure is known (i.e. matrix elements of electromagnetic transitions)
 - Straightforward method quantum-mechanical treatment: high number of partial waves, coupled channel equations... not very practical :(
 - Simplified and replaced by a semiclassical approach without a significant loss of accuracy

Simplified description of Coulomb excitation

- Projectile is moving along a hyperbolic orbit and excitation of nuclear states is caused by the time-dependent electromagnetic field between the collision partners
- The trajectories are described by the classical equations of motion, quantum mechanics is used to describe the effect of the electromagnetic field on the nucleus
- Other simplifying assumptions:
 - small energy transfer
 - interaction expanded in a multipole series and only monopole-multipole terms taken into account
 - time separation of the collision $(10^{-19}s)$ and deexcitation process $(>10^{-13}s)$

Validity of classical trajectories

 trajectories can be described by the classical equations of motion, excitation process is described using quantum mechanics.



- semiclassical treatment is expected to deviate from the exact calculation by terms of the order $\sim 1/\eta$: most important systematic error in Coulomb-excitation analysis

Limitation to monopole-multipole terms

The excitation process can be described by the time-dependent Hamiltonian H:

 $H = H_P + H_T + V(r(t))$

 $H_{\mathsf{P}/\mathsf{T}}$: free Hamiltonian of the projectile/target nucleus

V(t) : time-dependent electromagnetic interaction

If the wave function is expressed by eigenfunctions of the free $H_{\text{P}/\text{T}}$:

$$\psi(\mathsf{t}) = \sum_{\mathsf{n}} \mathsf{a}_{\mathsf{n}}(\mathsf{t}) \phi_{\mathsf{n}}$$

one gets a set of coupled equations for time-dependent excitation amplitudes $a_n(t)$

$$i\hbar \frac{da_{n}(t)}{dt} = \sum_{m} \langle \phi_{n} | V(t) | \phi_{m} \rangle \exp(i(E_{n} - E_{m})/\hbar) a_{m}(t)$$

Then V(t) can be expanded in multipoles:

$$\begin{split} \mathsf{V}(\mathsf{r}(\mathsf{t})) &= \mathsf{Z}_\mathsf{T} \mathsf{Z}_\mathsf{P} \mathsf{e}^2/\mathsf{r} & \text{monopole-monopole (Rutherford) term} \\ &+ \sum_{\lambda\mu} \mathsf{V}_\mathsf{P}(\mathsf{E}\lambda,\mu) + \sum_{\lambda\mu} \mathsf{V}_\mathsf{T}(\mathsf{E}\lambda,\mu) & \text{electric multipole-monopole excitation,} \\ &+ \sum_{\lambda\mu} \mathsf{V}_\mathsf{P}(\mathsf{M}\lambda,\mu) + \sum_{\lambda\mu} \mathsf{V}_\mathsf{T}(\mathsf{M}\lambda,\mu) & \text{magnetic excitation (small at low v/c)} \\ &+ \text{ higher order multipole-multipole terms (neglected - estimated at ~ 0.5 \%)} \end{split}$$

Multi-step excitation and coupled equations

$$i\hbar \frac{da_{n}(t)}{dt} = \sum_{m,\lambda} \langle \phi_{n} \| \hat{M} \lambda \| \phi_{m} \rangle \exp(i(E_{n} - E_{m})/\hbar) a_{m}(t) \qquad \hat{M} = E, M$$

- in heavy-ion induced Coulomb excitation the interaction strength gives rise to multiple excitation
- a nuclear state can be populated directly, via several intermediate states
- excitation probability of an individual state may depend on many matrix elements involved in different excitation paths
- high number of coupled equations for excitation amplitudes $\mathsf{a}_n(t)$
- dedicated data analysis codes needed

(excitation cross sections σ are Rutherford cross sections multiplied by the excitation probability $|a_n|^2$)



 10^{+}

Deexcitation process

For a given set of matrix elements $\langle \phi_n \| \hat{M} \lambda \| \phi_m \rangle$ the set of coupled equations

$$i\hbar \frac{da_n(t)}{dt} = \sum_{m,\lambda} \langle \phi_n \| \hat{M}\lambda \| \phi_m \rangle \exp(i(E_n - E_m)/\hbar) a_m(t)$$

is solved in order to determine level populations.

The same set of matrix elements describes the deexcitation process:

$$P(\hat{M}\lambda; I_i \to I_f) = \frac{8\pi(\lambda+1)}{\lambda((2\lambda+1)!!)^2} \cdot \frac{1}{\hbar} \cdot \left(\frac{E_{\gamma}}{\hbar c}\right)^{2\lambda+1} \cdot B(\hat{M}\lambda; I_i \to I_f)$$
$$B(\hat{M}\lambda; I_i \to I_f) = \frac{1}{2I_i+1} \langle I_f \| \hat{M}\lambda \| I_i \rangle^2$$

The calculation includes effects influencing γ -ray intensities: internal conversion, γ -ray angular distribution, its attenuation due to finite size of Ge detectors, deorientation

GOSIA code

GOSIA: Rochester - Warsaw semiclassical Coulomb excitation least-squares search code

Developed in early eighties by T. Czosnyka, D. Cline, C.Y. Wu (Bull. Am. Phys. Soc. 28 (1983) 745.) and continuously upgraded



Approximations used in GOSIA

- 1. semi-classical approximation
 - symmetrisation of the trajectory to take into account the energy transfer
- 2. limitation to the monopole-multipole term
- 3. other effects taken into account in the description of the excitation process:
- correction for the dipole polarisation effect: quadrupole interaction V(E2) multiplied by a factor

$$1 - d \cdot \frac{E_p A_t}{Z_t^2 (1 + A_p / A_t)} \frac{a}{r}$$

where d = 0.005 (empirical E1 polarisation strength, from photo-nuclear absorption cross section or GDR energy + dipole sum rule)

Alder and Winther, Coulomb excitation, appendix J

The default value seems to be inadequate for ligth nuclei, cf. M. Kumar Raju, PLB 777 (2018) 250. Otherwise a minor effect: 104 Ru – 10% change of population of 10^+_{γ} if effect increased 2 times (J. Srebrny, NPA 766, 25 (2006))

 integration over scattering angles covered by particle detectors and incident energy (beam stopping in the target) – changing meshpoints may give an effect of few %, especially for multi-step excitation

Effects taken into account when describing decay

- start from statistical tensors calculated in the excitation stage
 - information on excitation probability and initial sub-state population
- cascade feeding from higher-lying states
- deorientation of the angular distribution (due to recoil in vacuum): Brenn and Spehl two-state model:
 - ¹⁰⁴Ru 2% change of matrix elements if effect increased by 20%
- relativistic transformation of solid angles
- attenuation due to finite size of gamma-ray detectors
- simplified (cylindrical) detector geometry (see M. Schumaker et al, PRC 80, 044325 (2009) for an estimate of effects of this simplification)
- all approximations have usually an effect $\sim 5\%$ on gamma-ray intensities (often similar to statistical uncertainties, increasing with number of steps needed)
- uncertainties lower than this are rather suspicious (unless they reflect the precision of a lifetime measurement, but the quality of such measurement should also be verified)

Number of parameters versus number of data points

- number of matrix elements coupling low-lying states is higher than number of transitions observed in a Coulomb-excitation experiment
- some of them have much smaller influence on gamma-ray intensities than others
- even if angular dependence of cross sections is measured, often problem remains underdetermined
 - especially if E1, E3 matrix elements are declared, or for odd-mass nuclei – M1
- additional spectroscopic data needed
 - these data are not used to fix any of the parameters, but enter the χ^2 function exactly like gamma-ray intensities
- in rare very undetermined cases theoretical relations between the MEs may be used (which couplings are negligible, similar, etc...)

Global vs local minimum

Standard question: is this a unique solution, or maybe a different combination of matrix elements can reproduce the experimental data equally well?

Genetic Algorithm in GOSIA: JACOB (P.J. Napiorkowski)

GOSIA:

- often trapped in a local minimum
- various starting points have to be carefully checked (combinations of signs and magnitudes)
- only for very simple cases "plug and play"

JACOB:

- scan of the χ^2 surface, "promising" minima localised
- integration procdure repeated for each of them, real solutions identified
- alternative method for error estimation (in development)