Nuclear reactions Approximations and Models

D. Bazin

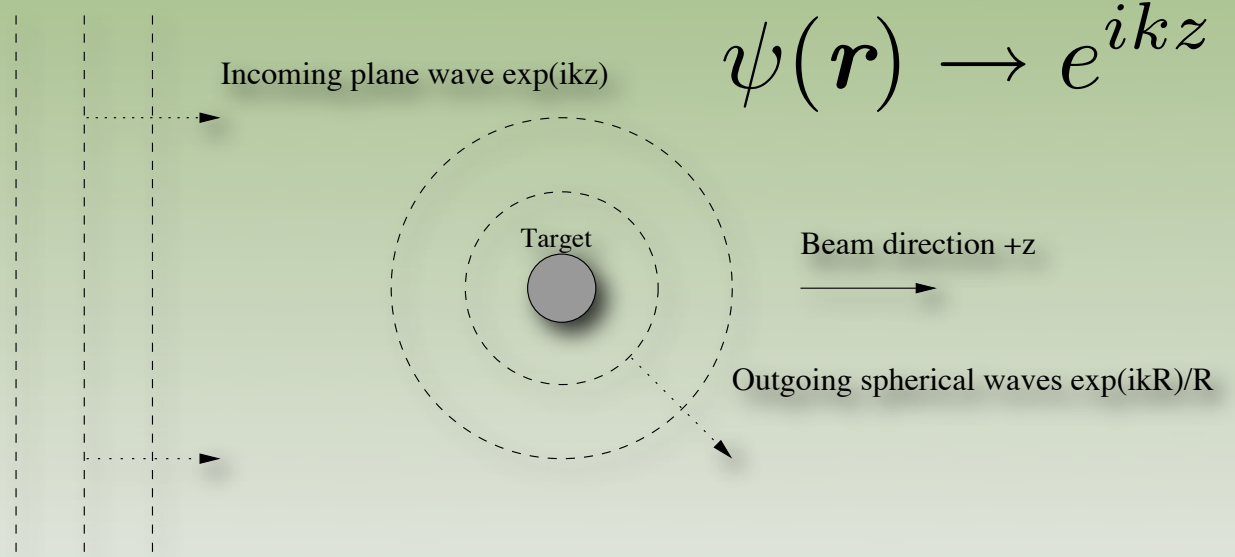
Lecture 2

Menu du jour

- Approximations
  - Born
  - DWBA
  - Semi-classical, WKB
  - Eikonal, Glauber
- Models
  - Optical model
  - Coupled-channels
  - Cluster models
  - Phenomenological models

Potential scattering theory

- Asymptotic Wave Function for elastic scattering
  - Incoming plane wave
  - Outgoing spherical wave
  - Scattering amplitude f



$$\psi(\boldsymbol{r}) \rightarrow e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$

- Cross section $\sigma = \dfrac{\text{number of particles emitted from a given reaction}}{(\text{number of incident particles})(\text{number of target nuclei/unit area})}$
  - Measure of the probability that a given reaction takes place
  - For instance: 1 particle/second out of 10^6 incident particles/second from a 1 mg/cm^2 ^{12}C target corresponds to 2.10^{-26} cm^2 or 20 mb
  - Differential cross section for elastic scattering: $\dfrac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2$
- For any reaction channel ß: A(a,b)B
  - Take internal degrees of freedom of particles into account
  - Total wave function:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\psi_a\psi_A + \sum_\beta f_\beta(\theta,\phi)\frac{e^{ik_\beta r_\beta}}{r_\beta}\psi_b\psi_B$$

$$\frac{d\sigma_\beta}{d\Omega} = \frac{v_\beta}{v_\alpha}|f_\beta(\theta,\phi)|^2$$

Schrödinger equation

- Simplified form: $$(\nabla^2 + k^2)\psi(\mathbf{r}) = U(\mathbf{r})\psi(\mathbf{r})$$
  - where: $k = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad U(\mathbf{r}) = \frac{2mV(\mathbf{r})}{\hbar^2}$
- Free particle solution: plane wave

$$U(\mathbf{r}) = 0 \rightarrow (\nabla^2 + k^2)\psi_0(\mathbf{r}) = 0 \rightarrow \psi_0(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

- Solution: plane wave + spherical waves generated by U

$$\psi(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int \frac{ik|\mathbf{r} - \mathbf{r}'|}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}')\psi(\mathbf{k}, \mathbf{r}')d\mathbf{r}'$$

Asymptotic limit

- The potential vanishes at large values of r: $\lim_{r\to\infty} U(\mathbf{r}) = 0$
  - simplifying for $r' \ll r$: $\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{r}$ $\quad k|\mathbf{r}-\mathbf{r}'| = kr - \mathbf{k}'\cdot\mathbf{r}'$
  - where the vector k′ has magnitude k and direction of r
- Asymptotic solution

$$\lim_{r\to\infty} \psi(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{e^{ikr}}{4\pi r}\int e^{-i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\psi(\mathbf{k},\mathbf{r}')d\mathbf{r}'$$

- Scattering amplitude

$$f(\theta,\phi) = -\frac{1}{4\pi}\int e^{-i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\psi(\mathbf{k},\mathbf{r}')d\mathbf{r}'$$

Born approximation

- Previous solution only formal: still contains unknown WF
  - Assume the potential U(r) is small: scattered wave has small amplitude and can be replaced by first term (plane wave)

$$f_{BA}(\theta,\phi) = -\frac{1}{4\pi}\int e^{-i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'}d\mathbf{r}'$$

  - Or: $f_{BA}(\theta,\phi) = -\frac{1}{4\pi}\int e^{i\mathbf{q}\cdot\mathbf{r}'}U(\mathbf{r}')d\mathbf{r}'$
  - where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ is the momentum transfer
  - Born approximation is a first order perturbation approximation

Distorted-wave Born approximation (DWBA)

- Two potential formulation
  - Split the potential into elastic and non-elastic parts:
$$U = U_{elas} + U_{other}$$
  - Suppose we know the solution of the elastic equation
$$(\nabla^2 + k^2)\psi_{elas}(\mathbf{r}) = U_{elas}(\mathbf{r})\psi_{elas}(\mathbf{r})$$
  - as outgoing waves (+) and incoming (time reversed) waves (-)
$$\psi^{(+)}_{elas}(\mathbf{k},\mathbf{r}) \qquad \psi^{(-)}_{elas}(\mathbf{k},\mathbf{r}) = \psi^{(+)}_{elas}(-\mathbf{k},\mathbf{r})^*$$
- The asymptotic solution can be expressed as
$$\lim_{r\to\infty} \psi(\mathbf{k},\mathbf{r}) = \psi^{(+)}_{elas}(\mathbf{k},\mathbf{r}) - \frac{e^{ikr}}{4\pi r}\int \psi^{(-)}_{elas}(\mathbf{k}',\mathbf{r}')^* U_{other}(\mathbf{r}')\psi(\mathbf{k},\mathbf{r}')d\mathbf{r}'$$
- and the scattering amplitude
$$f(\theta,\phi) = f_{elas}(\theta,\phi) - \frac{1}{4\pi}\int \psi^{(-)}_{elas}(\mathbf{k}',\mathbf{r}')^* U_{other}(\mathbf{r}')\psi(\mathbf{k},\mathbf{r}')d\mathbf{r}'$$

- Use Born approximation: elastic channel dominates reaction
  - Use "distorted waves" of elastic scattering instead of plane waves

$$f_{DWBA}(\theta,\phi) = f_{elas}(\theta,\phi) - \frac{1}{4\pi}\int \psi^{(-)}_{elas}(\mathbf{k}',\mathbf{r}')^* U_{other}(\mathbf{r}')\psi^{(+)}_{elas}(\mathbf{k},\mathbf{r}')d\mathbf{r}'$$

- Generalization to any two-body reaction A(a,b)B

$$f_{DWBA}(\theta,\phi) = -\frac{1}{4\pi}\int \psi^{(-)}_{\beta}(\mathbf{k}_\beta,\mathbf{r}_\beta)^* \langle b,B|U_{other}|a,A\rangle \psi^{(+)}_{\alpha}(\mathbf{k}_\alpha,\mathbf{r}_\alpha)d\mathbf{r}_\alpha d\mathbf{r}_\beta$$

  - elastic amplitudes for both entrance and exit channels has to be known!
  - usually calculated from optical potential fitted on elastic scattering data
  - non-elastic reaction potential determined by reaction model

Partial waves decomposition

- Motivation
  - Central scattering potential: angular momentum constant of motion
  - Wave function for a given angular momentum can factorize:

$$\psi_{\ell m}(\mathbf{r}) = u_\ell(r) Y_\ell^m(\theta, \phi)$$

  - Simplify 3D Schrödinger equation into series of 1D radial equations

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 w_\ell}{\mathrm{d}r^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right] w_\ell = E w_\ell$$

with: $w_\ell(r) = r u_\ell(r)$

centrifugal barrier

- Partial waves expansion of plane wave (free particle solution)

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)j_{\ell}(kr)P_{\ell}(\cos(\theta))$$

  - Radial part are spherical Bessel function which asymptotically behave as sum of incoming and outgoing spherical waves:

$$\lim_{kr\to\infty} j_{\ell}(kr) = \frac{\sin(kr - \frac{1}{2}\ell\pi)}{kr} = \frac{i^{1-\ell}}{2kr}\left[(-1)^{\ell}e^{-ikr} - e^{ikr}\right]$$

- Asymptotic form of radial WF for a given partial wave
  - Elastic channel: $\lim_{r\to\infty} u_{\ell,\alpha}(r) = \frac{y_{\ell}}{r}\left[(-1)^{\ell}e^{-ik_{\alpha}r} - S_{\ell,\alpha}e^{ik_{\alpha}r}\right]$
  - Non-elastic channels: $\lim_{r\to\infty} u_{\ell,\beta}(r) = -\frac{y_{\ell}}{r}\sqrt{\frac{v_{\alpha}}{v_{\beta}}}S_{\ell,\beta}e^{ik_{\beta}r}$
  - Partial wave scattering amplitudes: $S_{\ell,\beta}$
  - Also called S-matrix scattering matrix elements

Scattering matrix and phase shifts

- Ensemble of scattering amplitudes for all reaction channels form a unitary scattering matrix:

$$\sum_{\beta} |S_{\ell,\beta}|^2 = 1$$

- The S-matrix can be expressed in terms of a phase shift, real for elastic scattering and complex for reactions:

$$S_\ell = e^{2i\delta_\ell} \qquad \lim_{r\to\infty} u_{\ell,\beta}(r) = (kr)^{-1}\sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell)$$

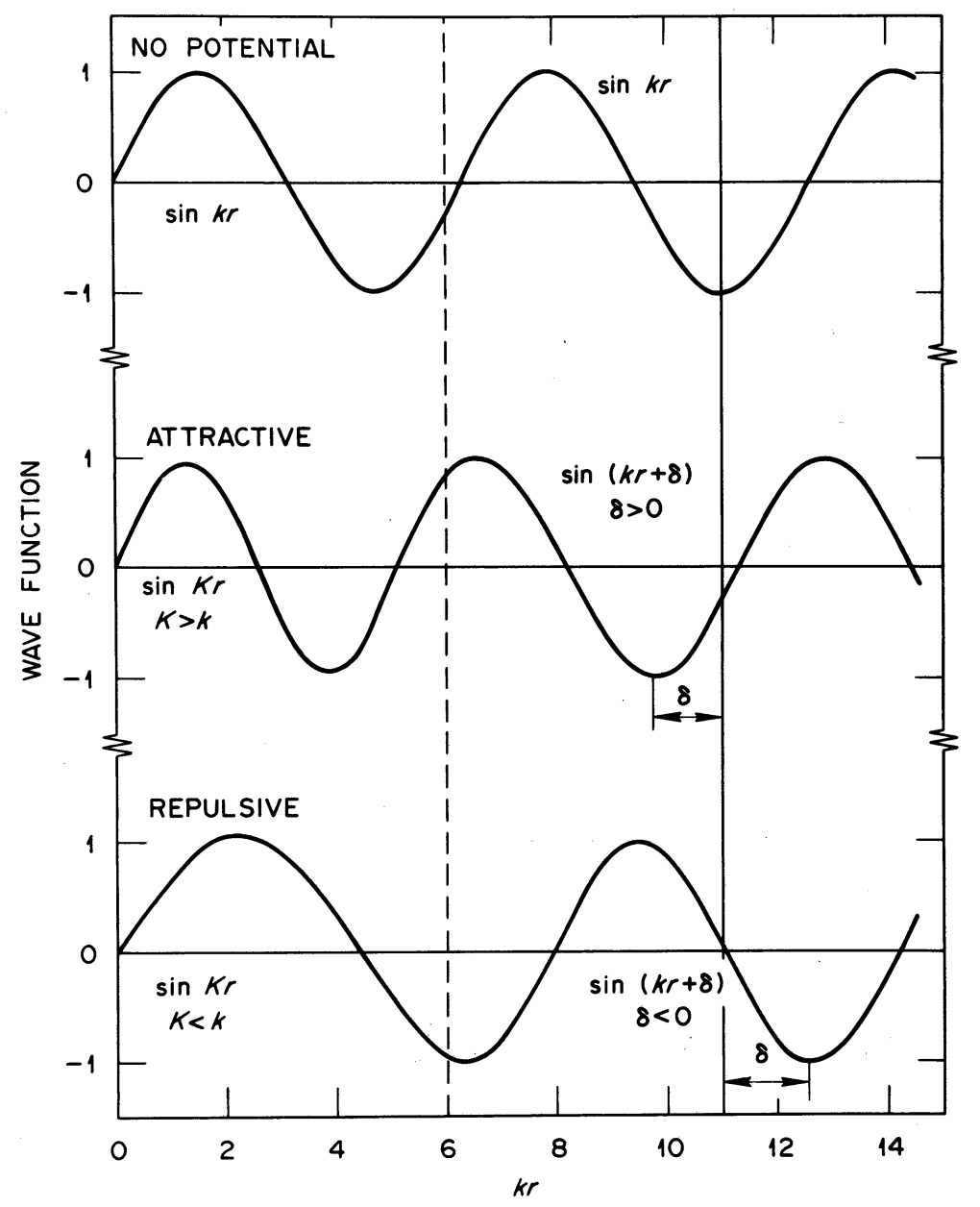
- The elastic and reaction cross sections:

$$\sigma_{el} = \frac{\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\,|S_\ell - 1|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

$$\sigma_r = \frac{\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)(1-|S_\ell|^2)$$

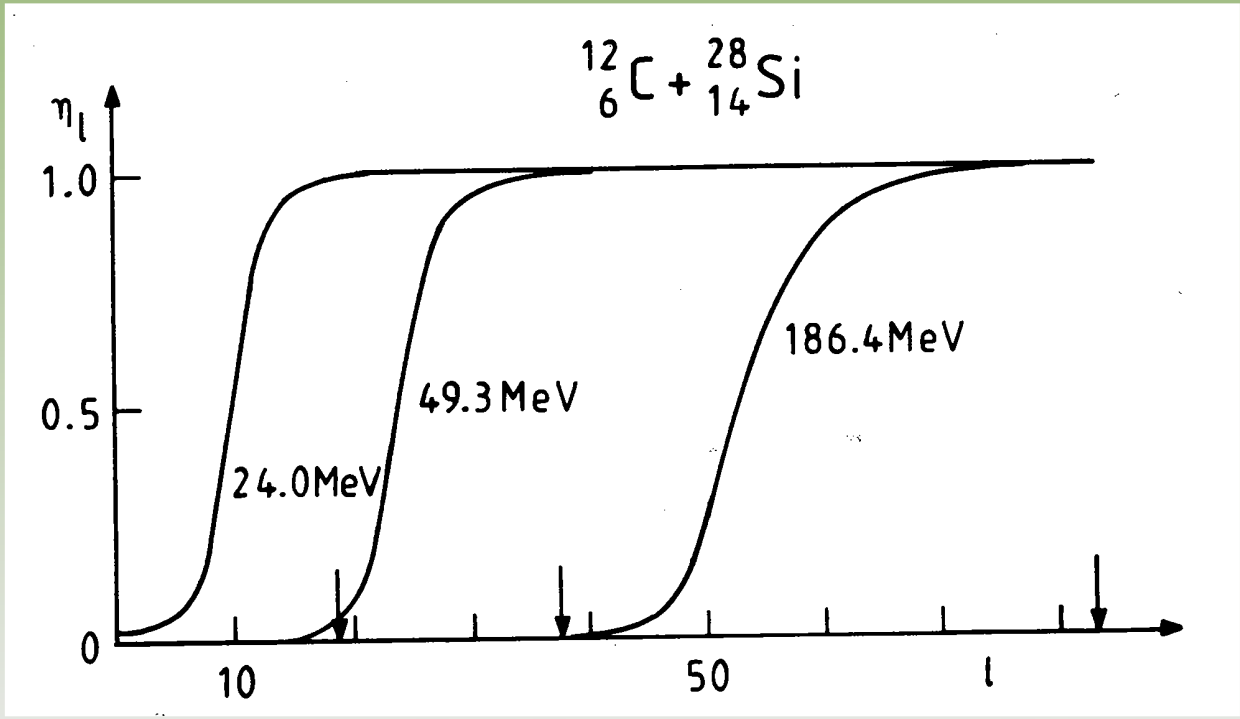
Illustration of phase shift

- Example of phase shift on S-wave by a square well potential (dash line)
- Attractive potential pulls wave function in, whereas repulsive potential pushes it out



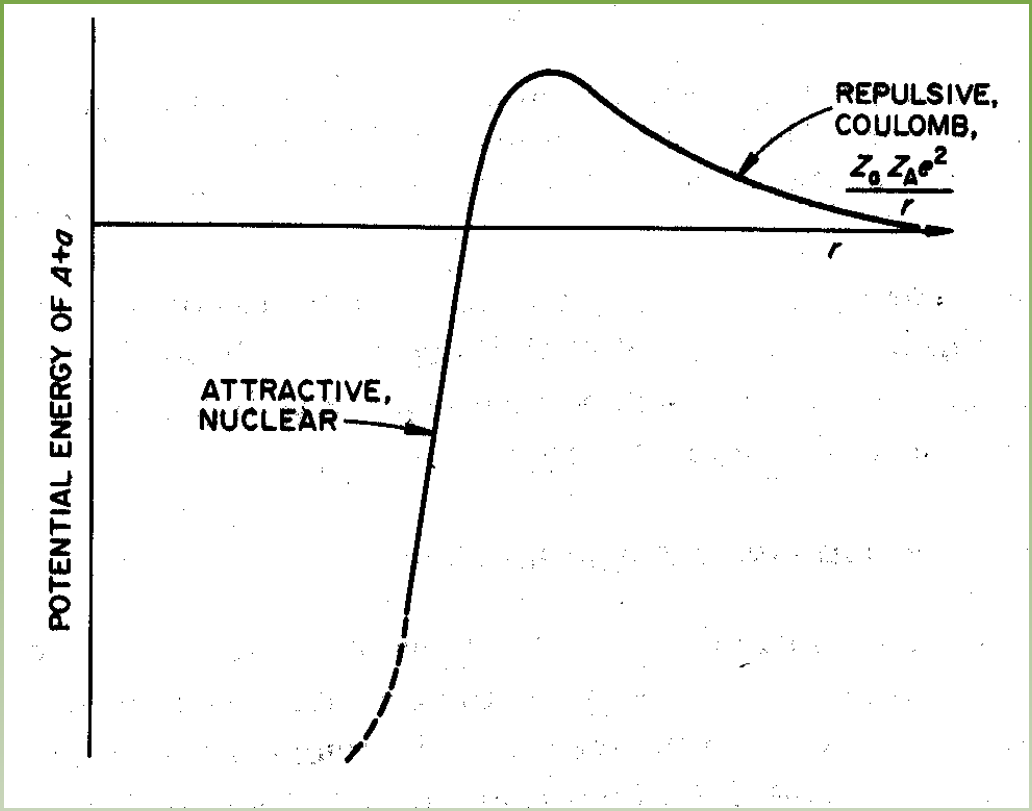
Partial wave summation

- How many partial waves contribute to the sum
  - Particles interact only for impact parameter $b \leqslant R_1 + R_2 = R$
  - Relative angular momentum $\ell\hbar = pb = \hbar kb$
  - The condition is then $\ell \leqslant kR$



Things omitted so far

- Coulomb effects
  - Coulomb barrier and long range
  - Elastic waves replaced by Coulomb waves in the entrance and exit channels
- Spin and isospin effects
  - Selection rules due to conservation of total angular momentum



Semi-classical approximations

- Validity and characteristics
  - Particle wavelength short (localized) compared to characteristic length of interacting system (i.e. nuclear radius or potential variation)
  - Motion of particles treated classically, but interaction treated quantum mechanically
- Implementations
  - WKB approximation: discrete sum over partial waves replaced by integration over angular momentum - Legendre polynomials replaced by their asymptotic form for large l.
  - Eikonal approximation: straight line trajectories further simplify integrals of WKB approximation

WKB approximation

- Requirements
  - Large number of partial waves contribute to the collision
  - Scattering amplitude varies slowly between l and l+hbar
- Phase shift

$$\delta_\ell^{\mathrm{WKB}} = (\ell + \tfrac{1}{2})\frac{\pi}{2} - kr_0 + \int_{r_0}^{\infty} \sqrt{\frac{2\mu}{\hbar^2}[E - V(r')] - \frac{\ell(\ell+1)}{r'^2}} - k\mathrm{d}r'$$

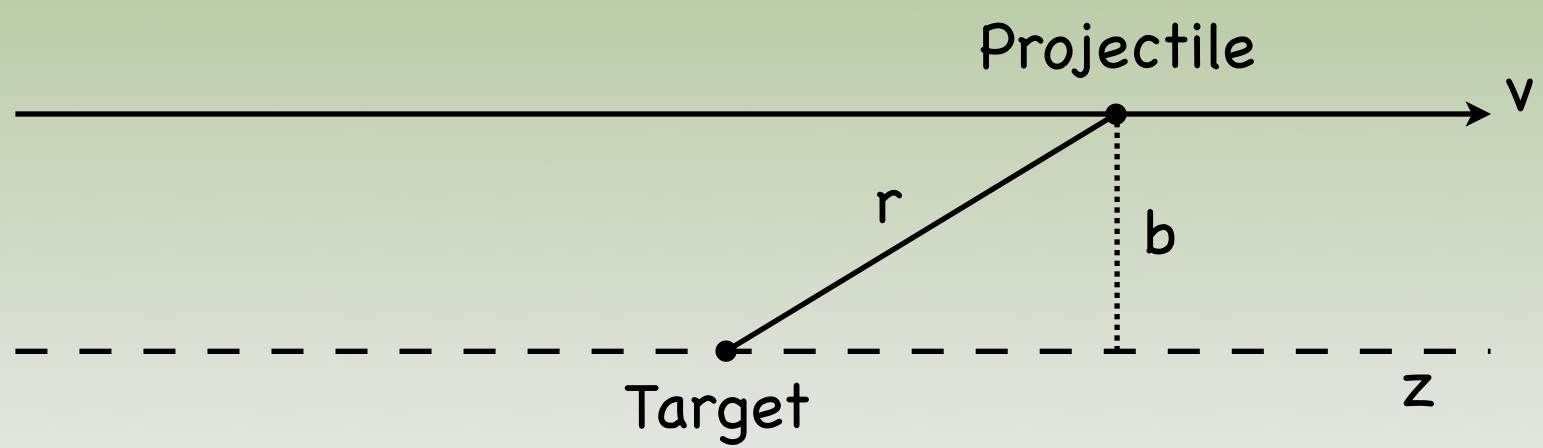
  - r_0 is the distance of closest approach
- Cross section equal to classical cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\theta} = \frac{b}{|\mathrm{d}\Theta/\mathrm{d}b|_\theta} \qquad \Theta(J) = 2\left(\frac{\mathrm{d}\delta_\ell^{\mathrm{WKB}}}{\mathrm{d}\ell}\right)_{\ell=(J-\frac{1}{2})/\hbar}$$

Eikonal approximation

- Energy of incident particle high: trajectory little deflected from a straight line
  - Distance of closest approach r_0 same as impact parameter b
  - Can get total (not partial) wave function and scattering amplitude
- Scattering amplitude

$$f^{\mathrm{E}}(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\int e^{i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r})e^{-ik\int_{-\infty}^{z}\frac{V(\mathbf{b}+z'\mathbf{k})}{2E}\mathrm{d}z'}\mathrm{d}\mathbf{r}$$



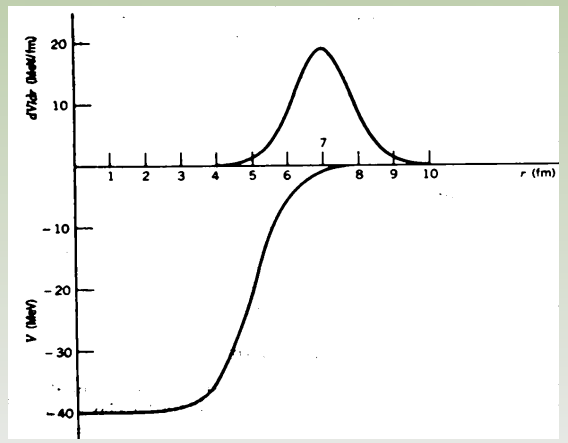
Optical model

- Basic assumptions
  - Scattering of structureless particles: potential scattering
  - Complex potential: imaginary part stands for all removals of flux from the elastic channel
- General form of the potential

$$U(r) = U_{\mathrm{R}}(r) + U_{\mathrm{I}}(r) + U_{\mathrm{D}}(r) + U_{\mathrm{S}}(r) + U_{\mathrm{C}}(r)$$

  - Real potential: $U_{\mathrm{R}}(r) = -V f_{\mathrm{WS}}(r, R, a)$
  - using a Wood-Saxon form factor:

$$f_{\mathrm{WS}}(r, R, a) = \frac{1}{1 + e^{\frac{(r-R)}{a}}}$$



- Absorption taken into account by two imaginary parts
  - Volume part: $U_{\mathrm{I}}(r) = -iW f_{\mathrm{WS}}(r, R_{\mathrm{I}}, a_{\mathrm{I}})$
  - Surface part: $U_{\mathrm{D}}(r) = 4ia_{\mathrm{I}}W_{\mathrm{D}}\frac{\mathrm{d}}{\mathrm{d}r}f_{\mathrm{WS}}(r, R_{\mathrm{I}}, a_{\mathrm{I}})$
  - Surface part dominates at low energy, but volume part becomes important at high energy (more penetration)
- Spin-orbit potential
  - Necessary to describe scattering of polarized particles

$$U_{\mathrm{S}}(r) = \mathbf{l}\cdot\mathbf{s}\left(\frac{\hbar}{m_\pi c^2}\right)^2 V_{\mathrm{S}}\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}f_{\mathrm{WS}}(r, R_{\mathrm{S}}, a_{\mathrm{S}})$$

- Coulomb potential

$$U_{\mathrm{C}}(r) = \frac{Z_1 Z_2 e^2}{2R_{\mathrm{C}}}\left(3 - \frac{r^2}{R_{\mathrm{C}}^2}\right)(r \leq R_{\mathrm{C}}), \frac{Z_1 Z_2 e^2}{r}(r > R_{\mathrm{C}})$$

- Total of 11 parameters to adjust from elastic scattering data:

$$V, R, a, W, W_{\mathrm{D}}, R_{\mathrm{I}}, a_{\mathrm{I}}, V_{\mathrm{S}}, R_{\mathrm{S}}, a_{\mathrm{S}}, R_{\mathrm{C}}$$

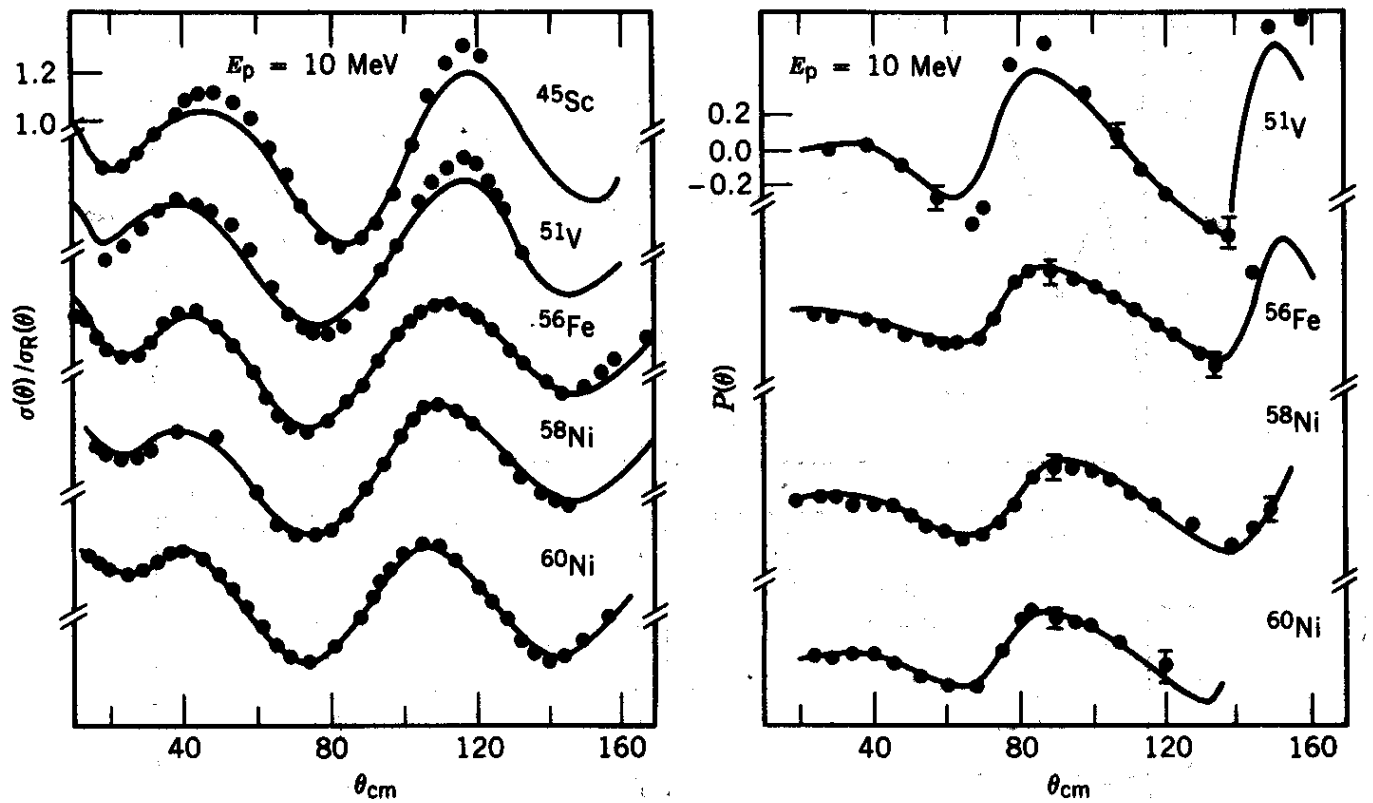
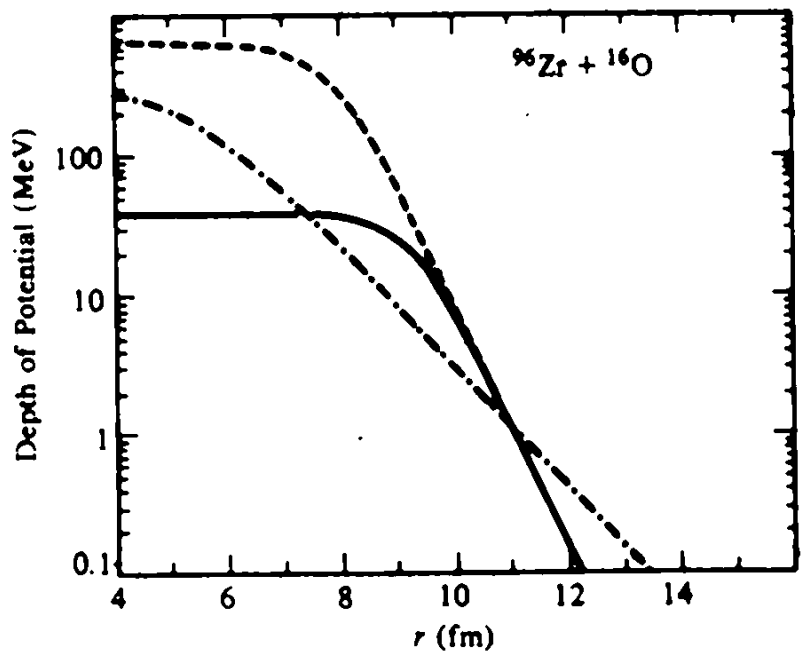


Figure 11.18 Optical-model fits to differential cross sections (at left, shown as a ratio to the Rutherford cross section) and polarizations, for 10-MeV protons scattered elastically from various targets. The solid lines are the fits to the data using the best set of optical-model parameters. From F. D. Becchetti, Jr., and G. W. Greenlees, *Phys. Rev.* **182**, 1190 (1969).

- Determination of optical potential parameters not necessarily unique

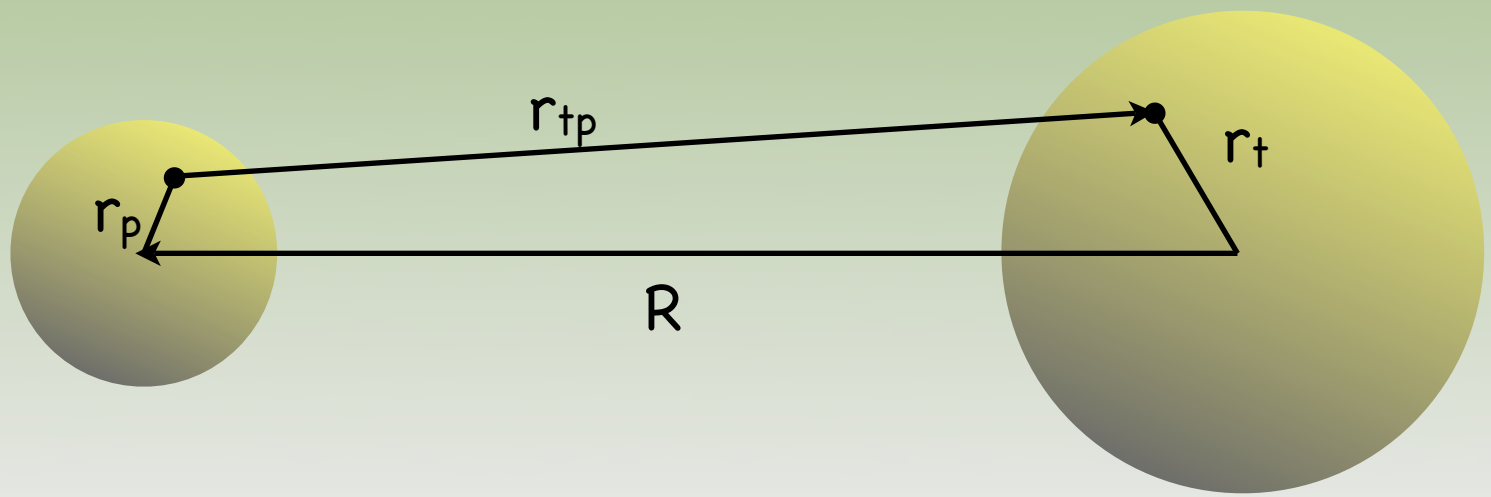


6.10. The real-part of the nuclear contribution to three optical model potentials which fit $^{16}O + {}^{96}Zr$ elastic scattering at $E_{lab}(^{16}O) = 60$ MeV. (From Becchetti, F. D. *et al.*, *Nucl. Phys.* **A203** (1973) 1.)

- Also use single and double folding potentials for real part
  - Use density distributions of projectile and target, and NN potential to calculate average interaction potential
  - Density distributions can come from other calculations such as HF

$$U(\mathbf{R}) = \int \rho_t(\mathbf{r}_t)\nu_{\mathrm{NN}}(\mathbf{r}_{tp})\mathrm{d}\mathbf{r}_t$$

$$U(\mathbf{R}) = \int\int \rho_p(\mathbf{r}_p)\rho_t(\mathbf{r}_t)\nu_{\mathrm{NN}}(\mathbf{r}_{tp})\mathrm{d}\mathbf{r}_p\mathrm{d}\mathbf{r}_t$$



Global optical potentials

- Motivation
  - Find parametrization of optical potential as a function of energy and target for a given projectile
  - For example: neutrons and protons from 1 keV to 200 MeV in the mass region 24 < A < 209 for spherical nuclei: A. J. Koning & J. P. Delaroche, Nucl. Phys. A 713 (2003) 231-310

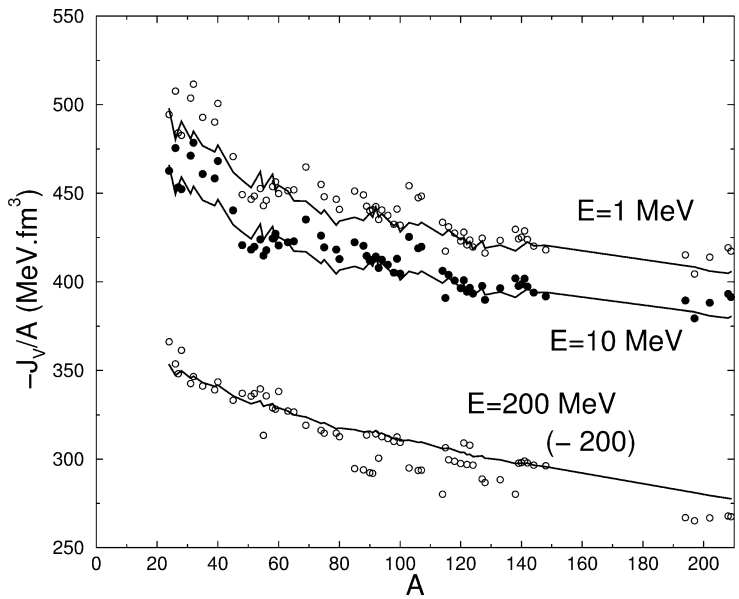


Fig. 48. Volume integrals for neutron-induced reactions for the real central potential as a function of mass, plotted at three different energies. The symbols correspond to the values of the local OMPs while the solid curves represent the global OMP (the curves in the deformed region, $148 < A < 194$ can be discarded).

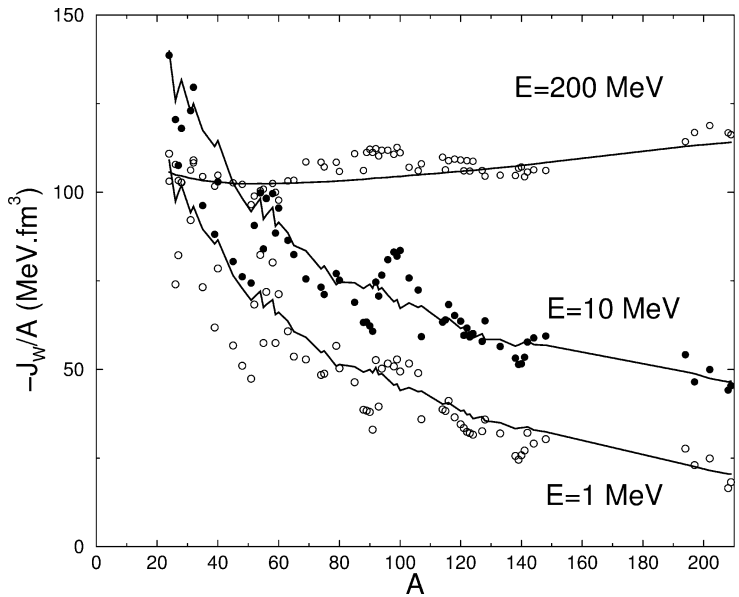


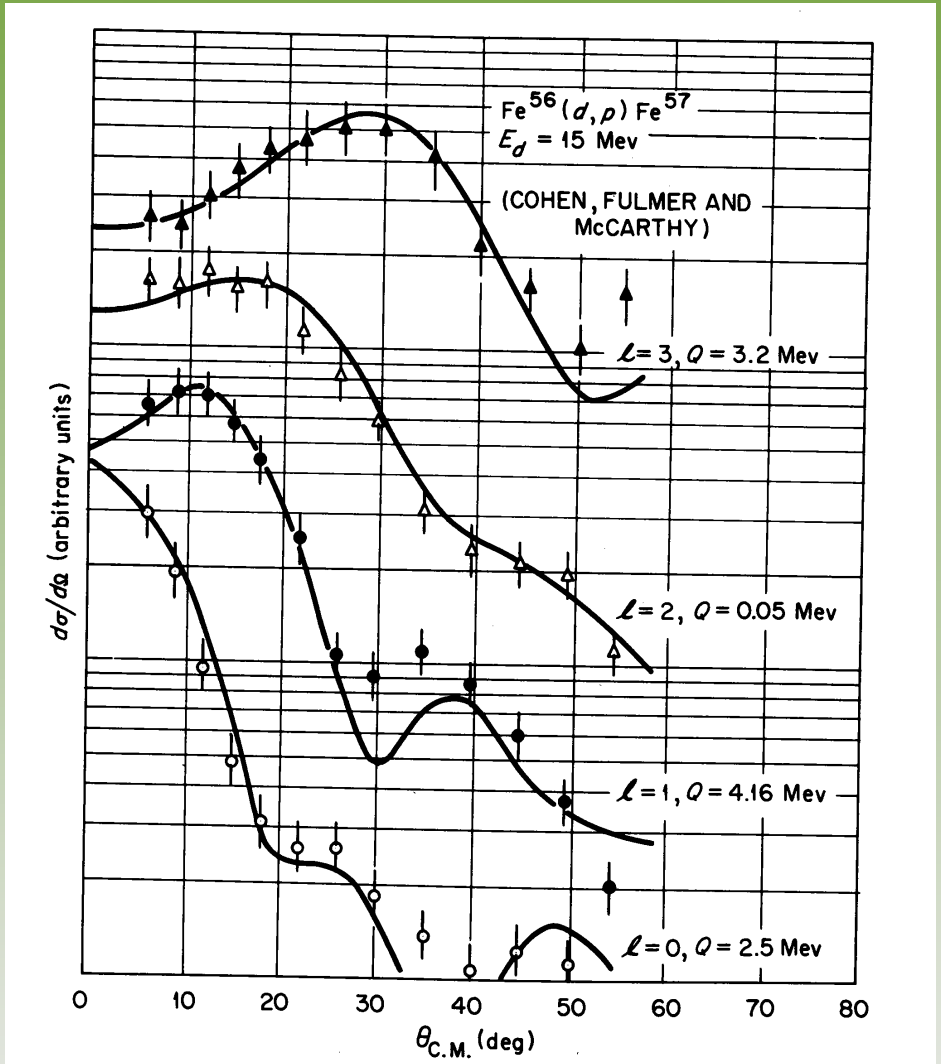
Fig. 49. Volume integrals for neutron-induced reactions for the imaginary central potential as a function of mass, plotted at three different energies. The symbols correspond to the values of the local OMPs while the solid curves represent the global OMP (the curves in the deformed region, $148 < A < 194$ can be discarded).

Transfer reactions

- Calculations done using the DWBA approximation
  - Need to know optical potentials for both entrance and exit elastic waves
  - When elastic scattering data is not available, one can use global optical potentials
  - Shape of differential cross section depends on angular momentum of the transfered nucleon (identification)
  - The calculations use partial wave decomposition - convergence obtained by increasing number of waves
  - Available codes: DW81, DWBA91-96-98, DWUCK4-5...
  - For example @ https://intra.nscl.msu.edu/programs

Example: $^{56}Fe(d,p)^{57}Fe$

- Position of cross section peak allows identification of l-value of transfered neutron
- Deduce spectroscopic information from comparison between experimental and single-particle DWBA cross sections



Spin-parity assignments

- Example: $^{36}S(d,p)^{37}S$ adds a neutron above N=20 in fp shell composed of single-particle $1f_{7/2}$, $2p_{3/2}$, $1f_{5/2}$ or $2p_{1/2}$ orbitals
- Spectroscopic factor S measures the weight of single-particle configuration in final state

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{exp}} = S'_{ij}\left(\frac{d\sigma}{d\Omega}\right)_{\text{DWBA}} \qquad S'_{ij} = \frac{2J_f+1}{2J_i+1}S_{ij} \qquad \sum_i S_{ij} = n_j$$

E (keV)	l	S'	S_1	S_2	J^π_1	J^π_2
0	3	7.328	0.916	~~1.221~~	$7/2^-$	~~$5/2^-$~~
646	1	2.796	0.699	~~1.398~~	$3/2^-$	~~$1/2^-$~~

Coupled-channels

- Direct reactions description uses first-order perturbation theory (Born approximation) assuming one-step process
- More complex reactions can proceed through multi-step processes depending on available paths and overlap between final and initial states

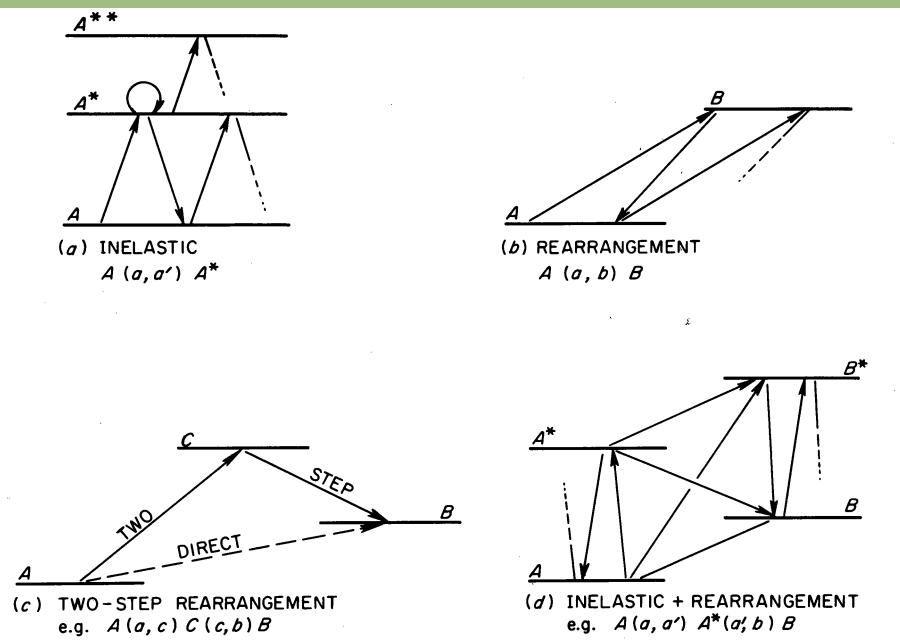
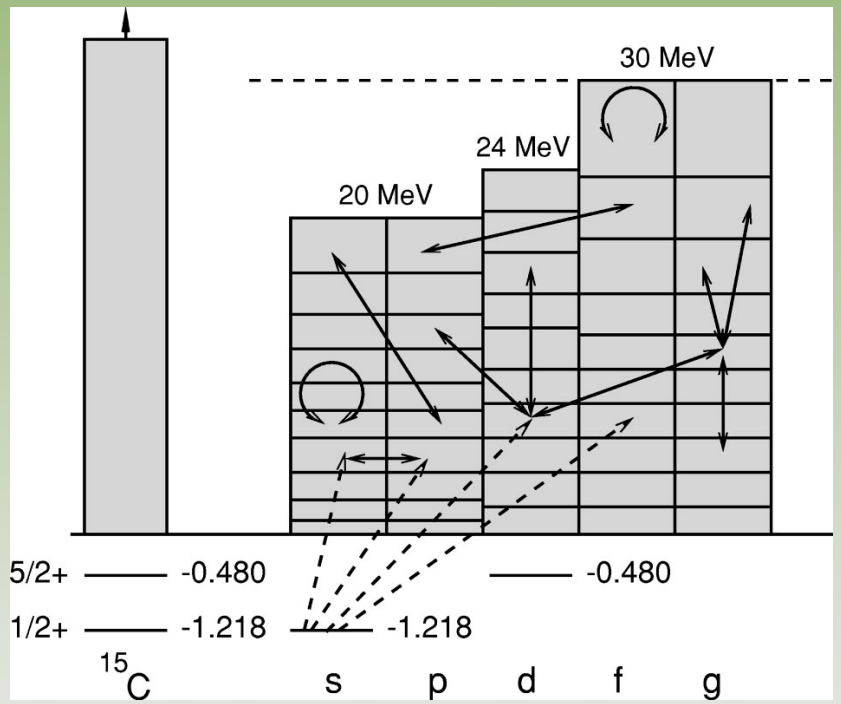


Figure 4.27 Illustrating various types of multi-step processes which may occur in direct reactions. Each arrow indicates one action by the interaction potential V. The Born approximation takes into account only one such arrow

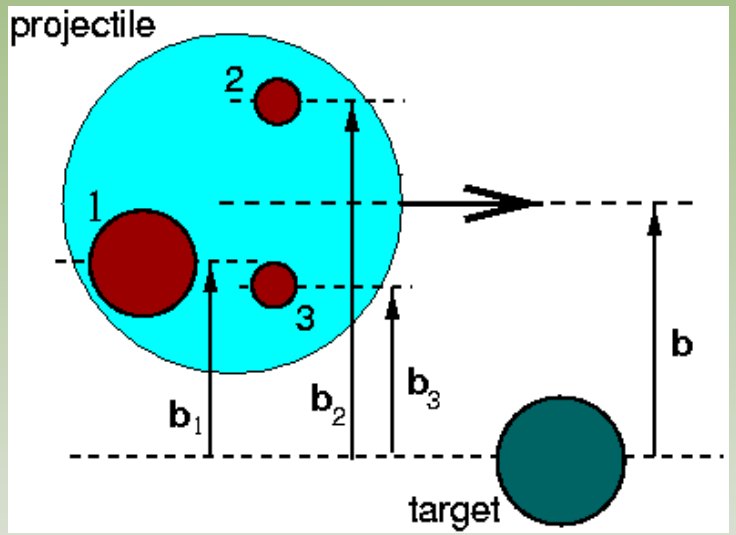
Coupling to the continuum: CDCC

- In particular for weakly bound nuclei, multi-step processes can couple to the continuum
- CDCC: Continuum Discretized Coupled Channels divide continuum states in chunks to perform CC calculation



Cluster models

- Motivation
  - Take explicitly into account the cluster structure of particular nuclei
  - Typical example of application: halo nuclei
- Few-body eikonal or Glauber theories
  - Applicable at high energy
  - Straight line trajectories
  - Removal of valence nucleons
  - Stripping component in knockout reactions (lecture 3)



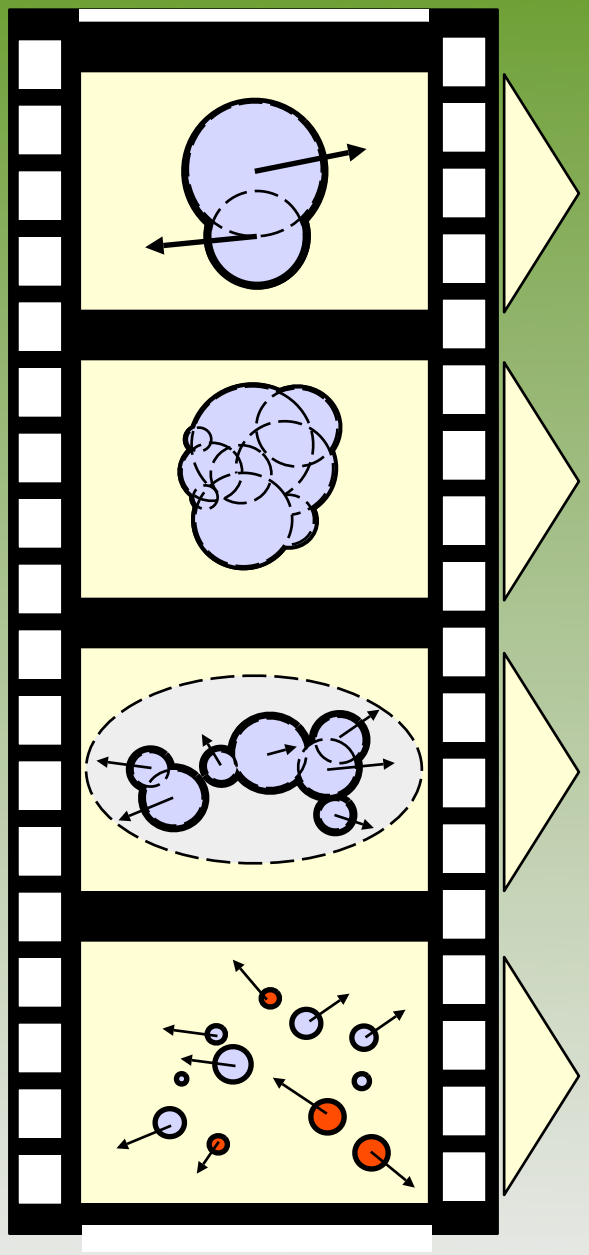
Complex reactions

- Low to intermediate energy: formation of compound nucleus by complete or incomplete fusion, followed by evaporation - deep-inelastic collisions
- High energy: depending on impact parameter, fragmentation or multi-fragmentation of both nuclei with formation of hot (participant) and cold (spectator) zones
- Phenomenological and statistical models better suited to deal with complexity and strong couplings which occur in this type of reactions
- Liquid-drop model
- BUU, AMD, ...

HIPSE: a minimal approach

- Heavy Ion Phase Space Exploration
- Created by D. Lacroix, D. Durand and A. Van Lauwe (PRC 69, 054604 (2004)
- Basic idea: macroscopic/microscopic simulation of heavy ion collisions at energies around the Fermi energy - event generator
- Simulation based on very simple rules (energy balance, barrier constraints, etc...) and random exploration of the phase space available during the collision
- Vast amount of data well reproduced by this model: complexity arise from simple rules and initial conditions (chaotic behavior)

Scenario



Entrance channel :
classical dynamics
of macroscopic clusters

Fast Nucleosynthesis in
a dense matter
from microscopic
nucleons properties

Out from the dense matter :
Important Final State Interaction

The after burn phase :
desexcitation of the initial
phase-space

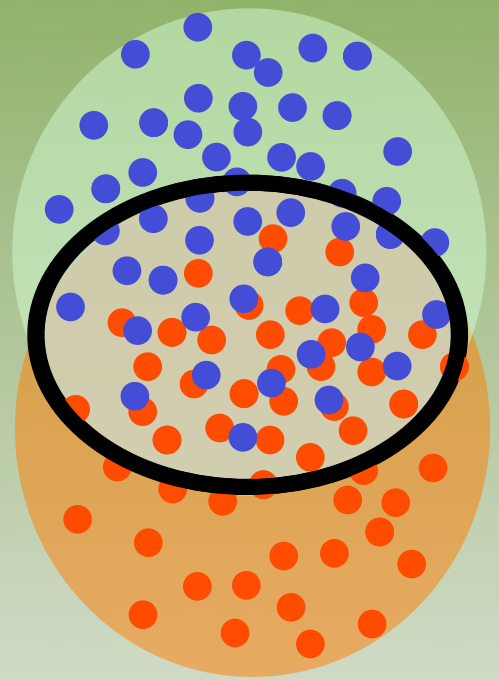
From: D. Lacroix (private communication)

Entrance channel

Participant-Spectator picture

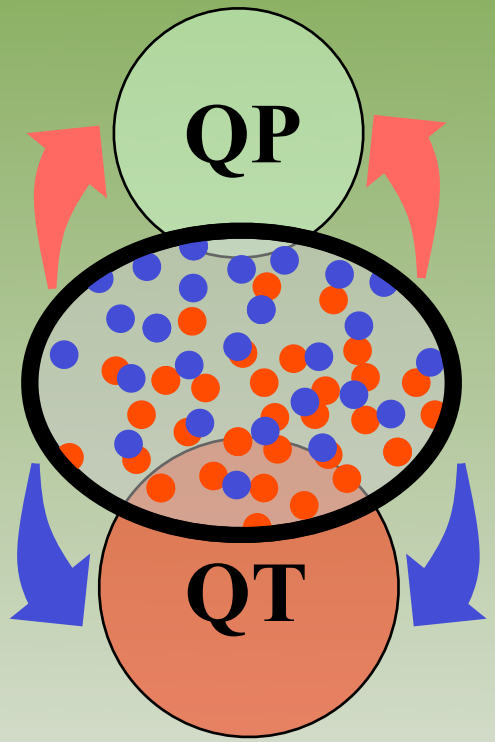
Importance of the geometry

Nucleon Sampling



Initial Fermi-motion
Frozen density approximation

Quasi-Participant Quasi-spectator

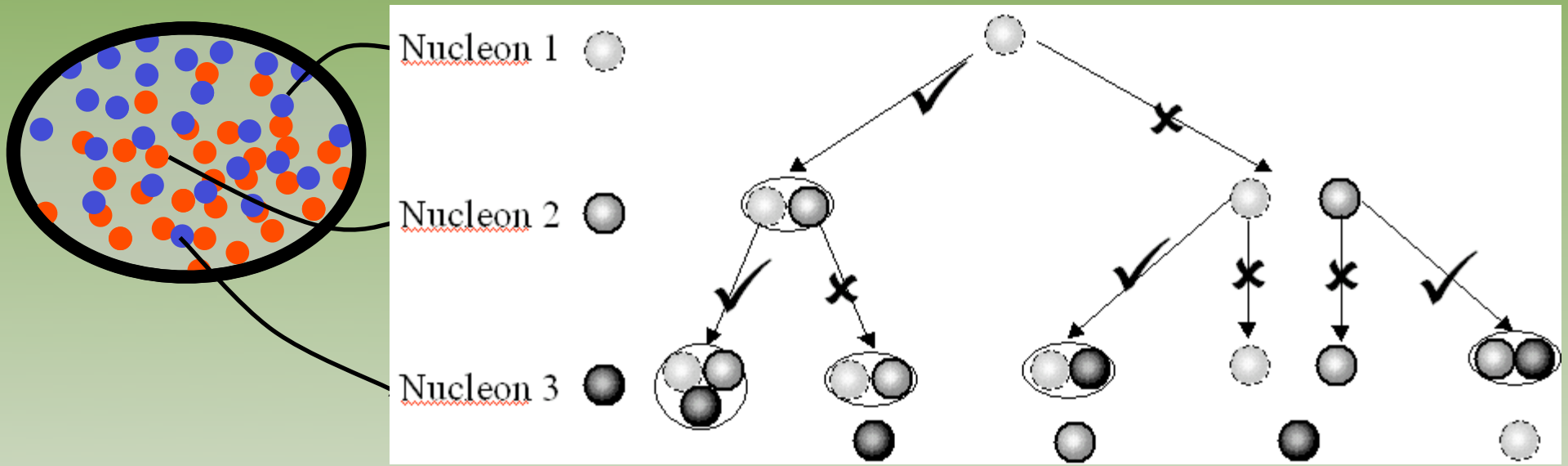


Exchange of particles

From: D. Lacroix (private communication)

Cluster synthesis in overlap region

- Phase space exploration: random exploration of most probable cluster formation



Coalescence conditions **1-existence** **2-proximity in position and momentum**

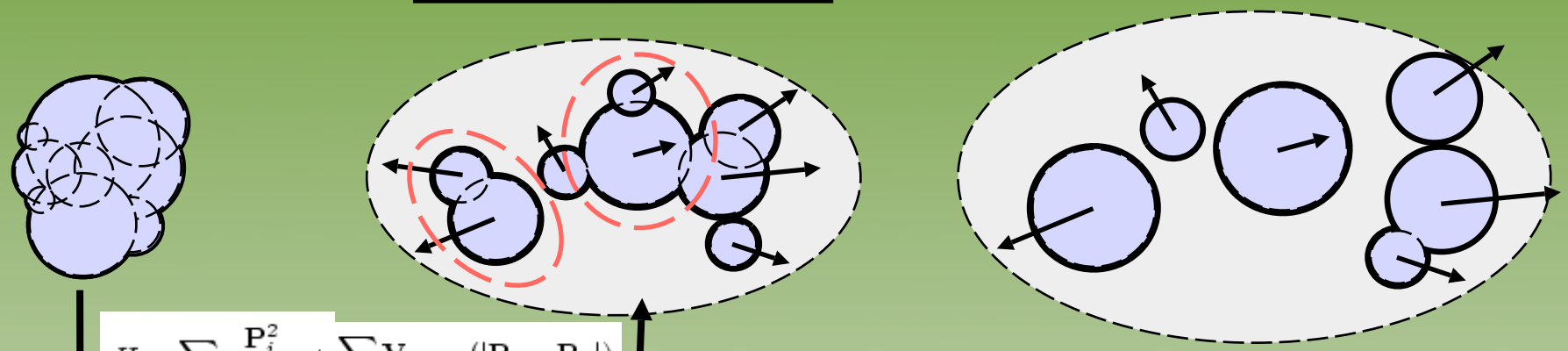
From: D. Lacroix (private communication)

Final state interaction

Initial partition

After the reaction time (*t=50 fm/c*) *test of fusion*

Before desexcitation $V_{pot} > 0$



$$H = \sum_i \frac{\mathbf{P}_i^2}{2mA_i} + \sum_{i<j} \mathbf{V}_{A_iA_j}(|\mathbf{R}_i - \mathbf{R}_j|)$$

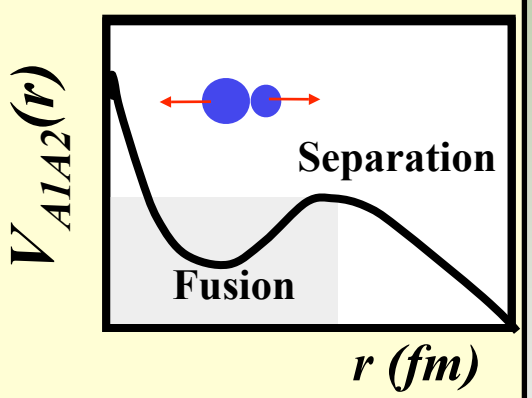
Classical dynamics

From nucleon motion we obtain :

N_{frag} **fragments**

$$\text{with} \begin{cases} (A_f, Z_f) \\ \mathbf{R}_f \\ \mathbf{P}_f \\ \mathbf{L}_f \end{cases}$$

Two-by-two Fusion test



Energy balance and sharing before desexcitation

$$E_0 = Q + E_K + E_{pot} + E^* + E_{rot}$$

This defines the phase-space before decay in-flight

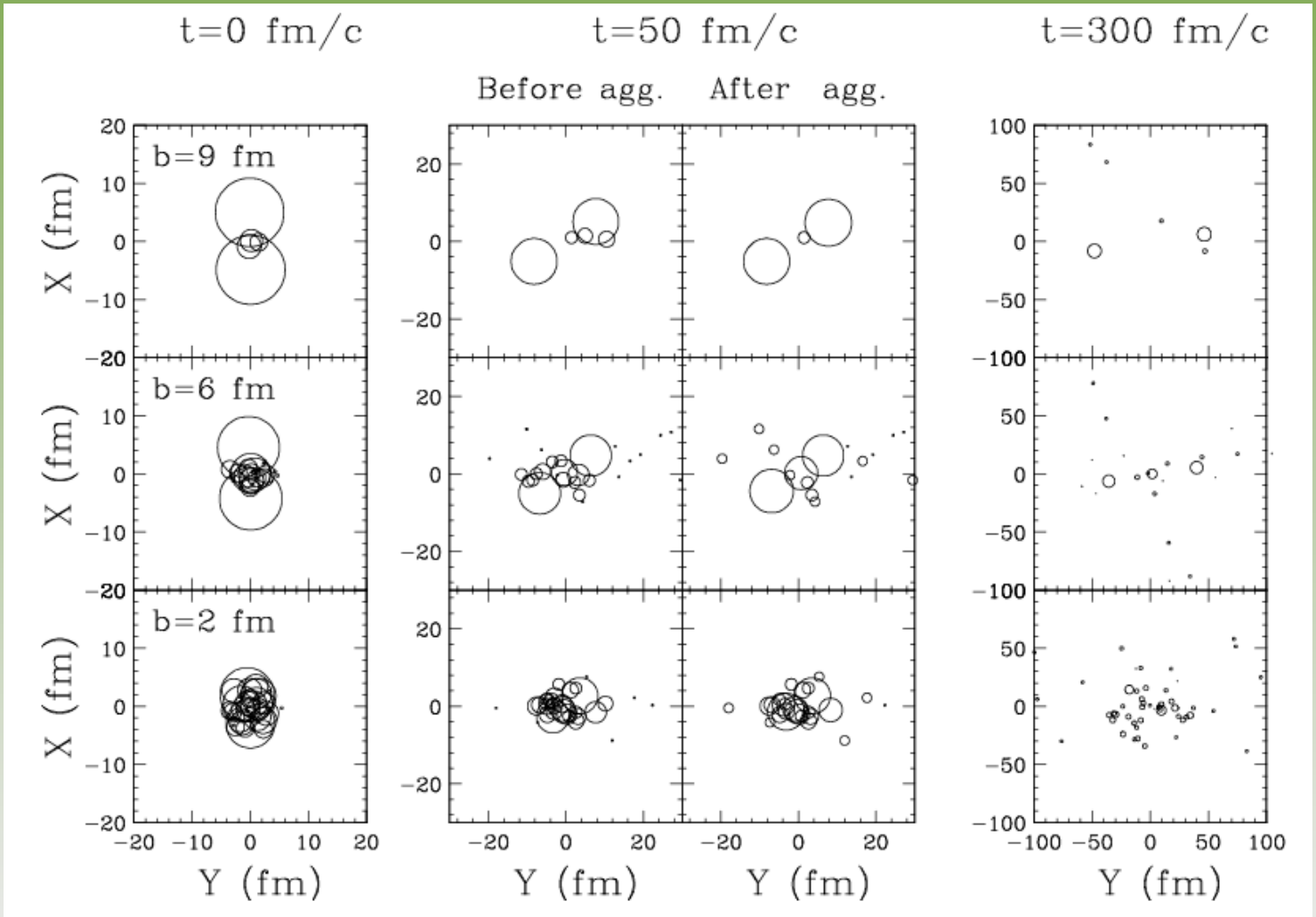
From: D. Lacroix (private communication)

Example: Xe+Sn @ 50 MeV/u

Maximum overlap

Final state interaction

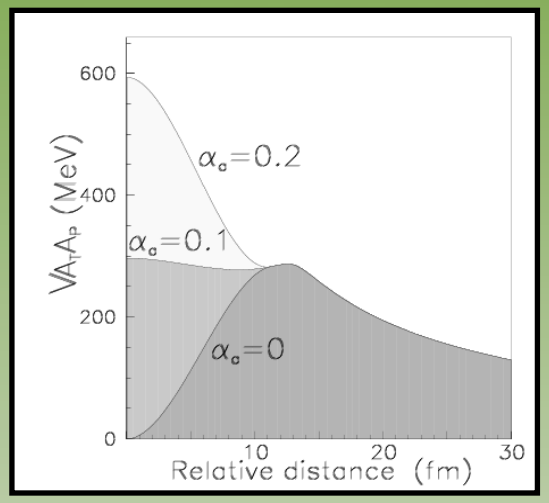
During the in-flight desexcitation



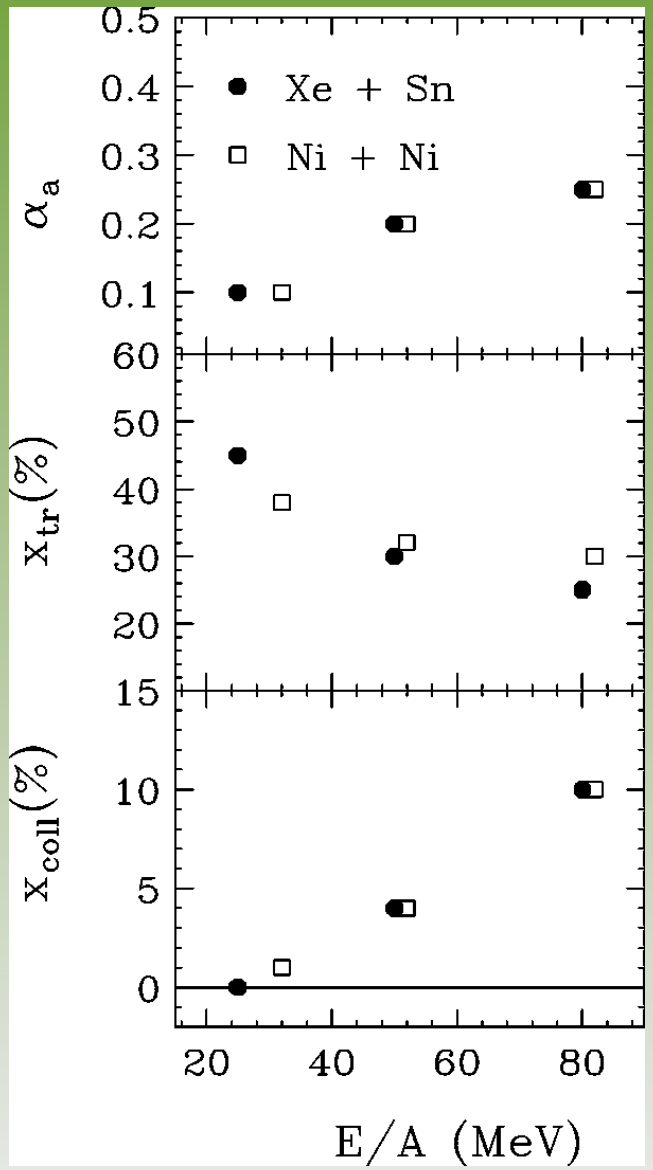
From: D. Lacroix (private communication)

Three parameters

- "Hardness" of potential as the target and projectile nuclei approach and overlap



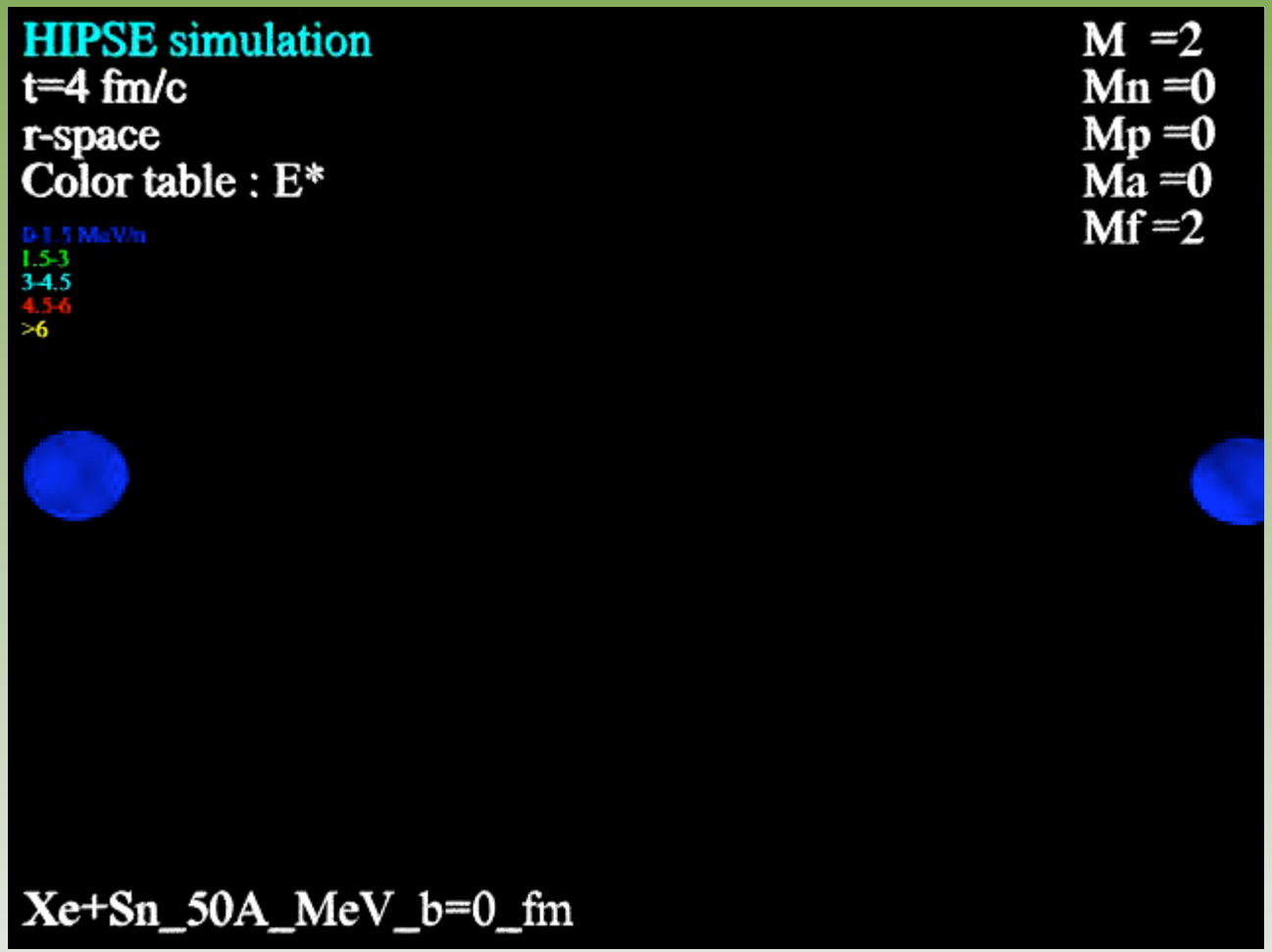
- Rate of exchange of particles between target and projectile
- Percentage of nucleon-nucleon collisions in the overlap region



From: D. Lacroix (private communication)

Example of one event

- Central collision of Xe + Sn at 50 MeV/u

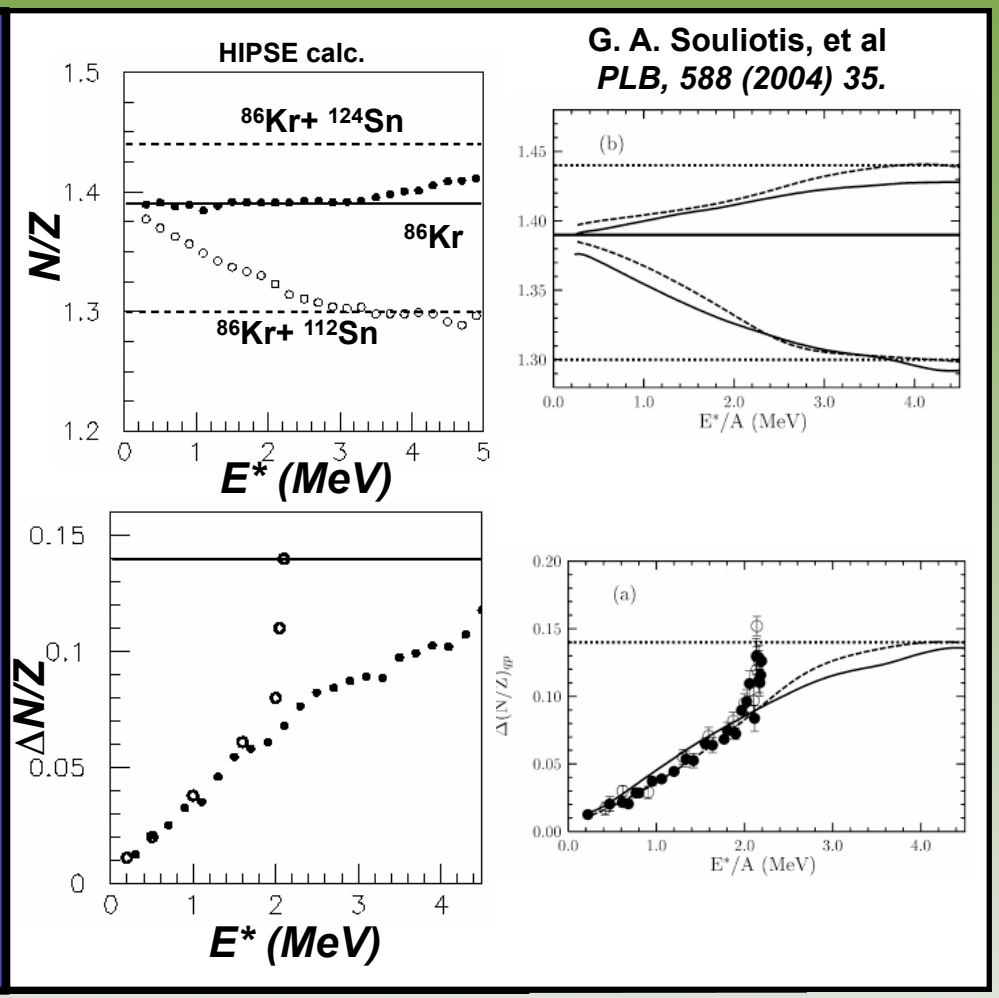


From: D. Lacroix (private communication)

Chemical and kinetic properties

INDRA DATA : Xe + Sn, 25,50,80 MeV/A

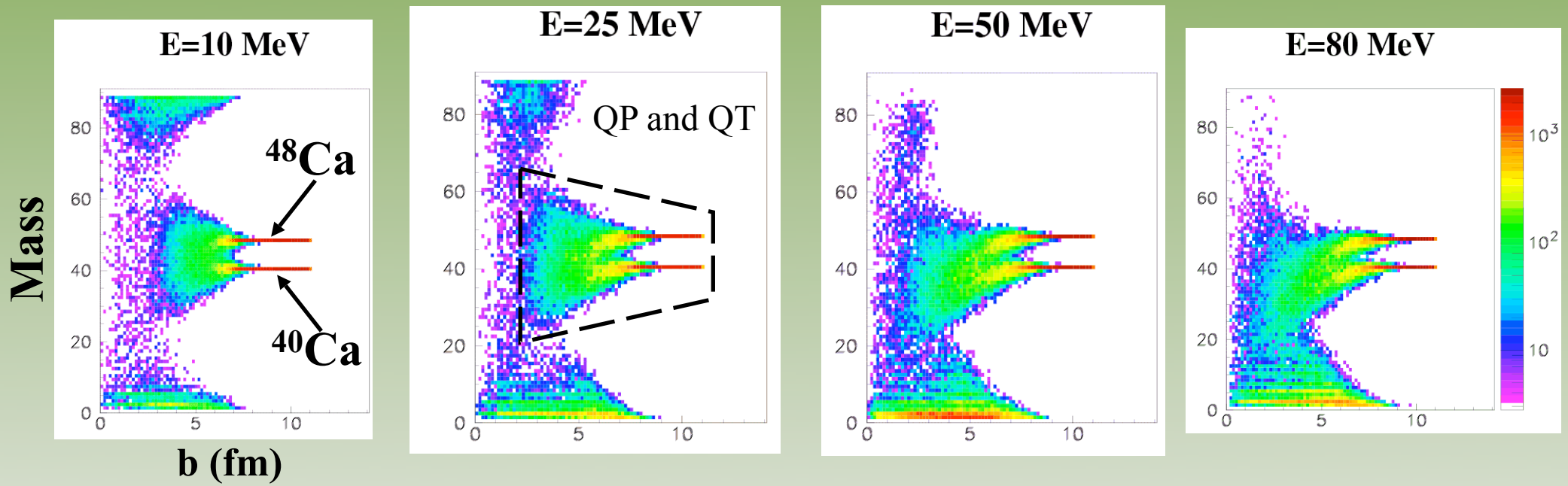
- Charge distribution ☺
- Mean kinetic energy ☺
- Fluctuations of kinetic energy ☺
- Parallel velocity ☺
- Angular distribution ☺
- Event by event correlations ☺
- Bimodality ☺
- Isospin effects ☺



From: D. Lacroix (private communication)

From compound to fragments

Fragment mass before desexcitation

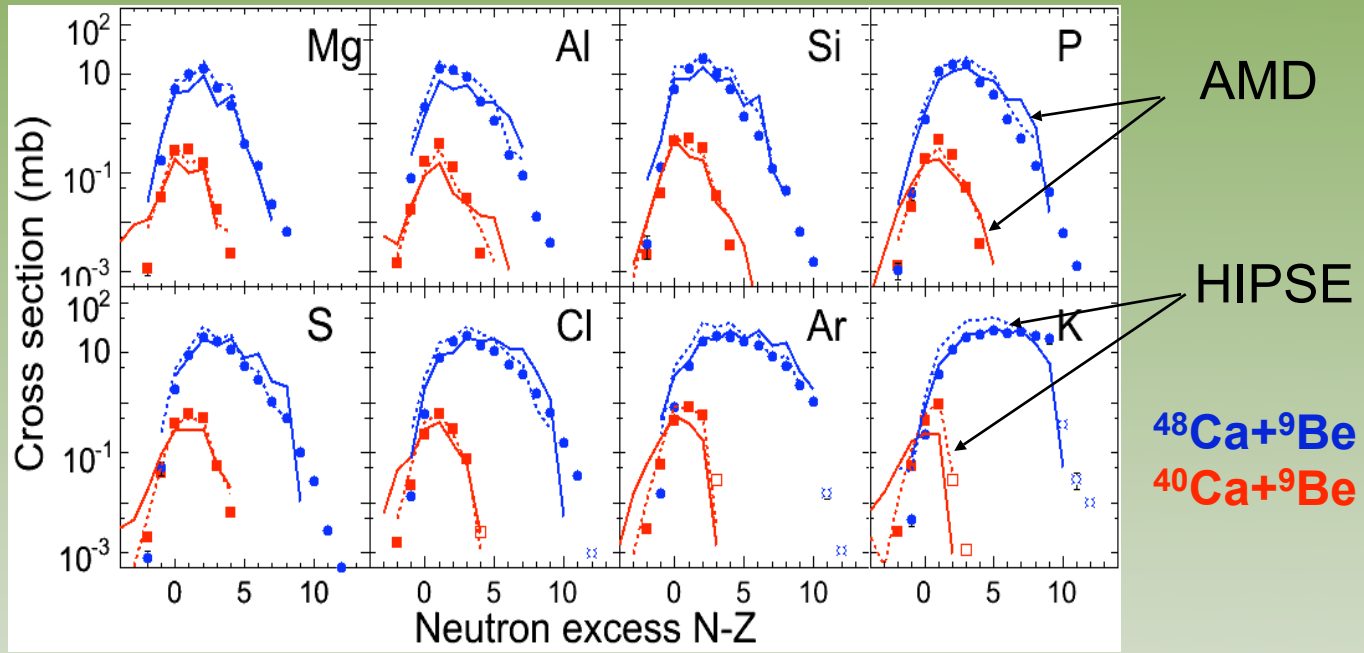


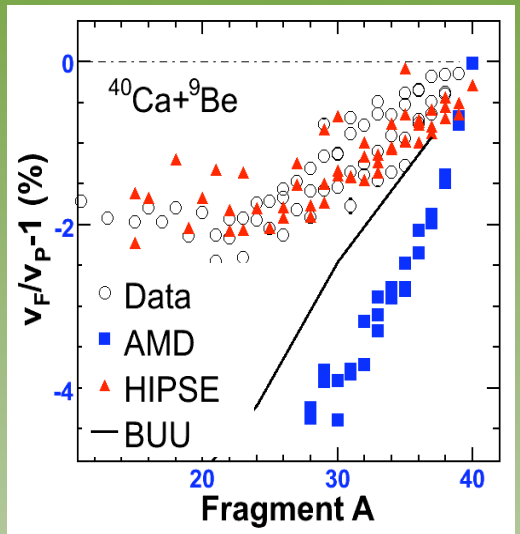
From: D. Lacroix (private communication)

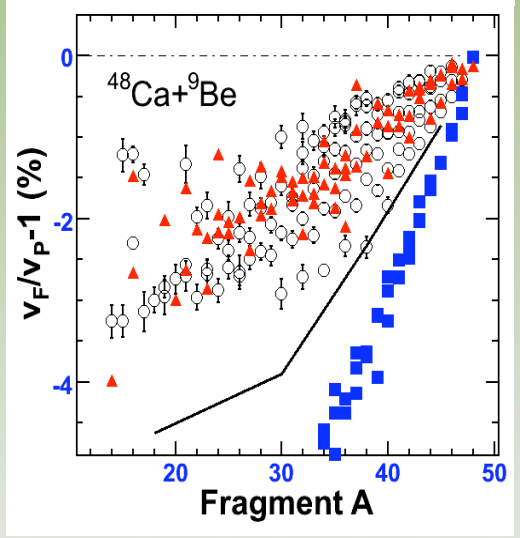
Application to projectile fragmentation

Production of Radioactive elements (HiRA Group)

M. Mocko (PhD Thesis)



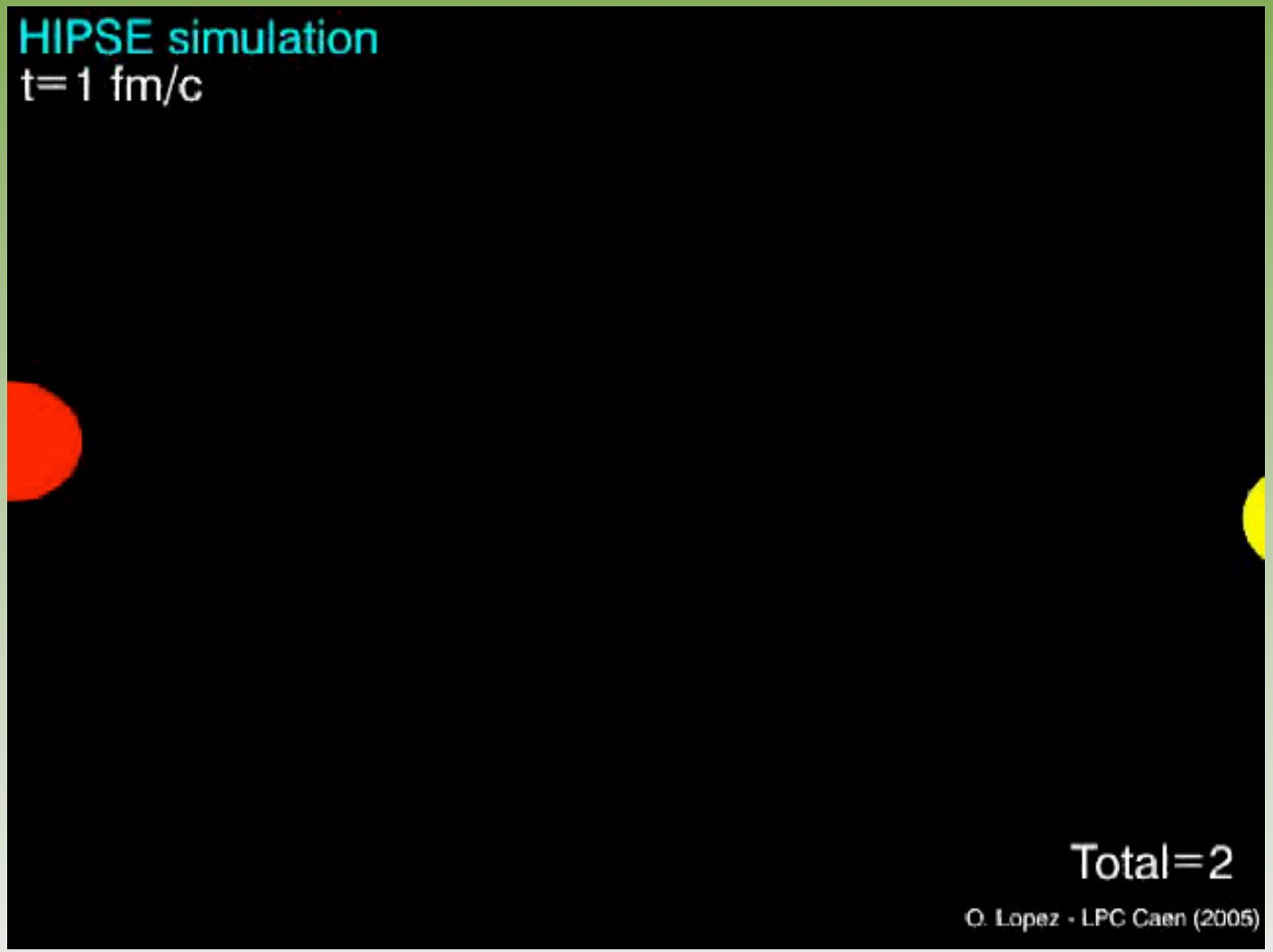




From: D. Lacroix (private communication)

Some more events…

- Peripheral collision of Xe+Sn at 50 MeV/u



From: D. Lacroix (private communication)

Availability

➡ **Two models with same ingredients have been developed and compared with success to experiments**

- **HIPSE for heavy-Ion reactions**
- **nIPSE for nucleon-Ion reactions**

A large set of data is now available… and could be compared with HIPSE.

http://caeinfo.in2p3.fr/theorie/theory_lacroix.html

Unix, Linux, Mac OS X

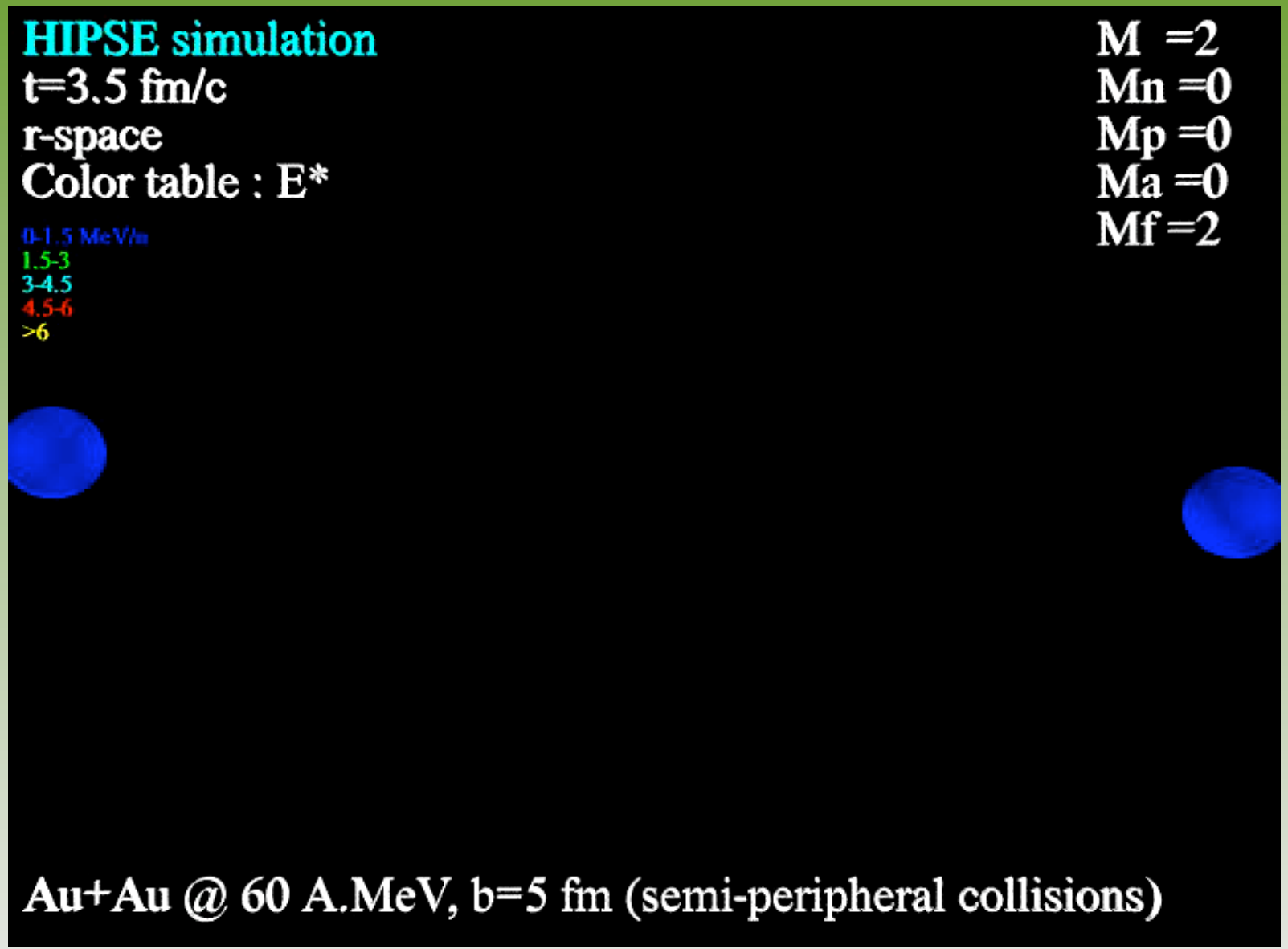
Ca+Ca	1	Million events per day
Xe+Sn	0.1	Million events per day
Au+Au	0.01	Million events per day

Thanks to

V. Blideanu, D. Durand, G. Lehaut, O. Lopez
A. Van Lauwe and E. Vient

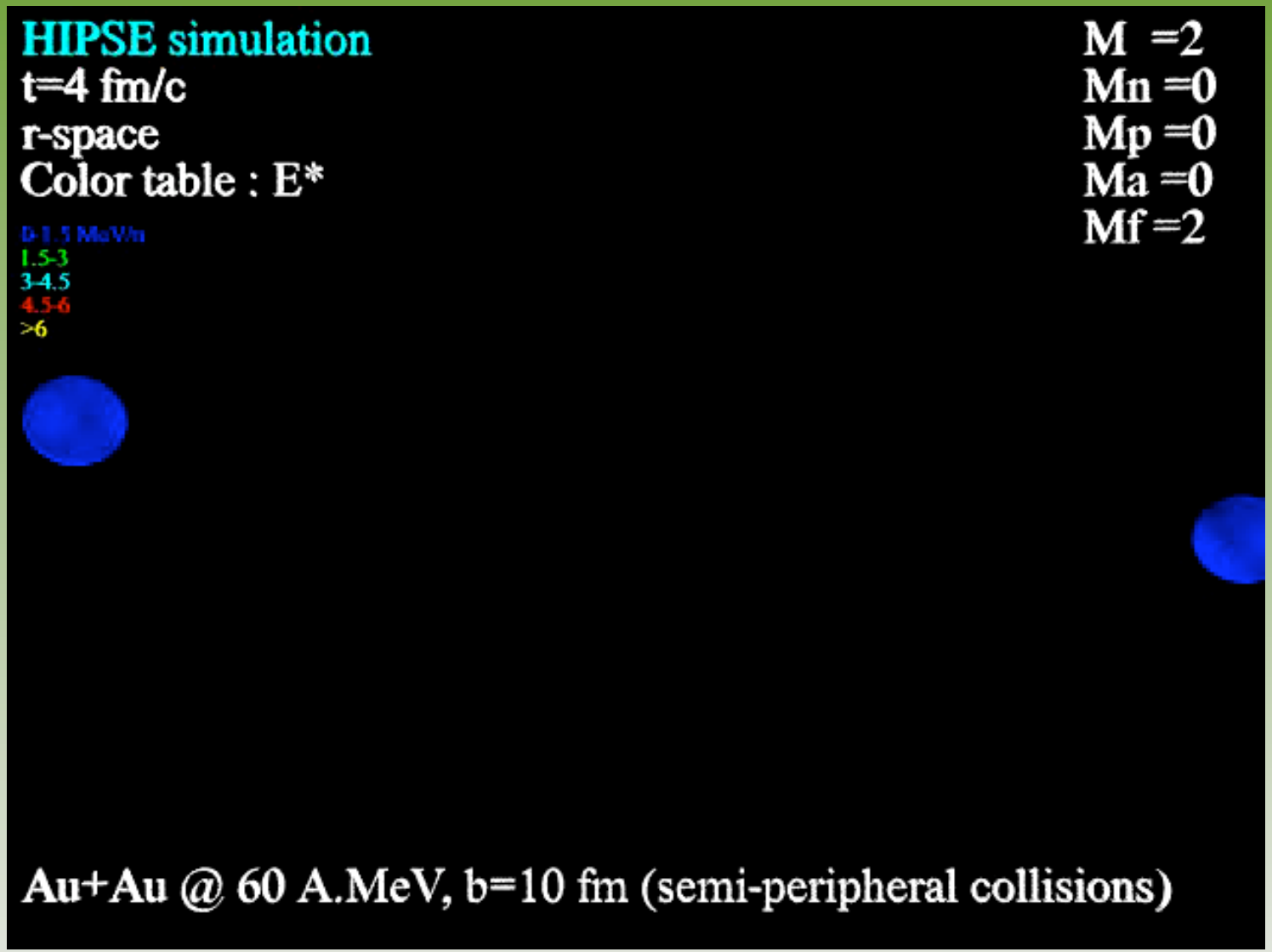
From: D. Lacroix (private communication)

More examples



From: D. Lacroix (private communication)

More examples (cont.)



From: D. Lacroix (private communication)