



the
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international centre for theoretical physics

SMR 1398/2

**WORKSHOP ON
NUCLEAR REACTION DATA AND NUCLEAR REACTORS:
PHYSICS, DESIGN AND SAFETY**

25 February - 28 March 2002

**Neutron Standards and
Basic Microscopic Theory**

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These are preliminary lecture notes, intended only for distribution to participants.

Neutron Standards and Basic Microscopic Theory

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Standard Neutron Cross Sections

Introduction to Potential Scattering

Neutron-Proton Scattering and N-N Interaction

R-Matrix Data Analysis

${}^3\text{He}(n, p){}^3\text{H}$ Reaction and Realistic Microscopic Models

${}^6\text{Li}$ - Neutron Scattering and Semi-Realistic Models

Conclusions

Standard Reactions

Light nuclei

$\text{H}(n, n)\text{H}$	1 keV – 20 MeV
${}^3\text{He}(n, p){}^3\text{H}$	thermal – 50 keV
${}^6\text{Li}(n, t){}^4\text{He}$	thermal – 1 MeV
${}^{10}\text{B}(n, \alpha){}^7\text{Li}$	thermal – 250 keV
${}^{10}\text{B}(n, \alpha, \gamma){}^7\text{Li}$	thermal – 250 keV
$\text{C}(n, n)\text{C}$	thermal – 1.8 MeV

Heavy nuclei

${}^{197}\text{Au}(n, \gamma)$	0.2 – 2.5 MeV
${}^{235}\text{U}(n, f)$	thermal – 20 MeV
${}^{238}\text{U}(n, f)$	threshold – 20 MeV

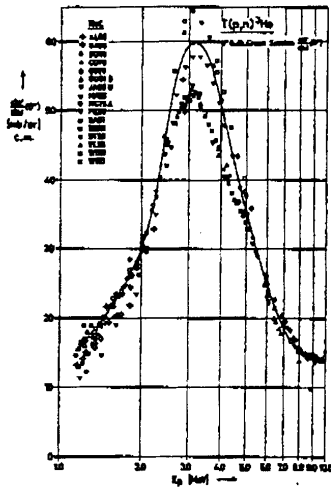
Theoretical treatment of light and heavy nuclei
vastly different

light nuclei	heavy nuclei
few well defined open channels	many, unspecified
few (broad) resonances	many, narrow
center-of-mass motion important	unimportant
detailed microscopic models	bulk properties
"Few Nucleon regime"	"Nuclear matter"

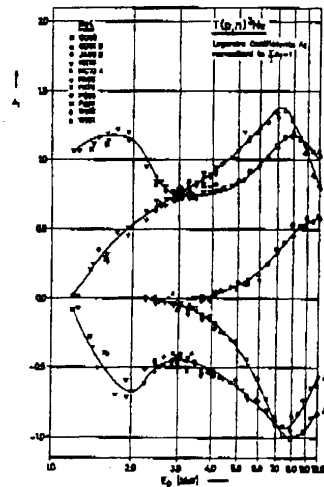
See typical examples

Neutron Production Cross Section $T(p, n)^3\text{He}$

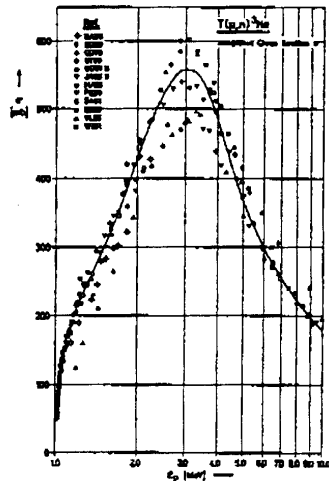
$T(p, n)^3\text{He}$. $\sigma(0^\circ \text{ c.m.})$, Legendre Coefficients, $\sigma(\text{total})$
Recommended and Experimental Values



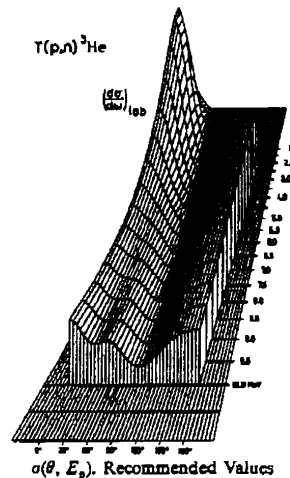
$\sigma(0^\circ \text{ c.m.})$. Experimental and Recommended Values



Legendre Coefficients
Experimental and Recommended Values



$\sigma(\text{total})$. Experimental and Recommended Values

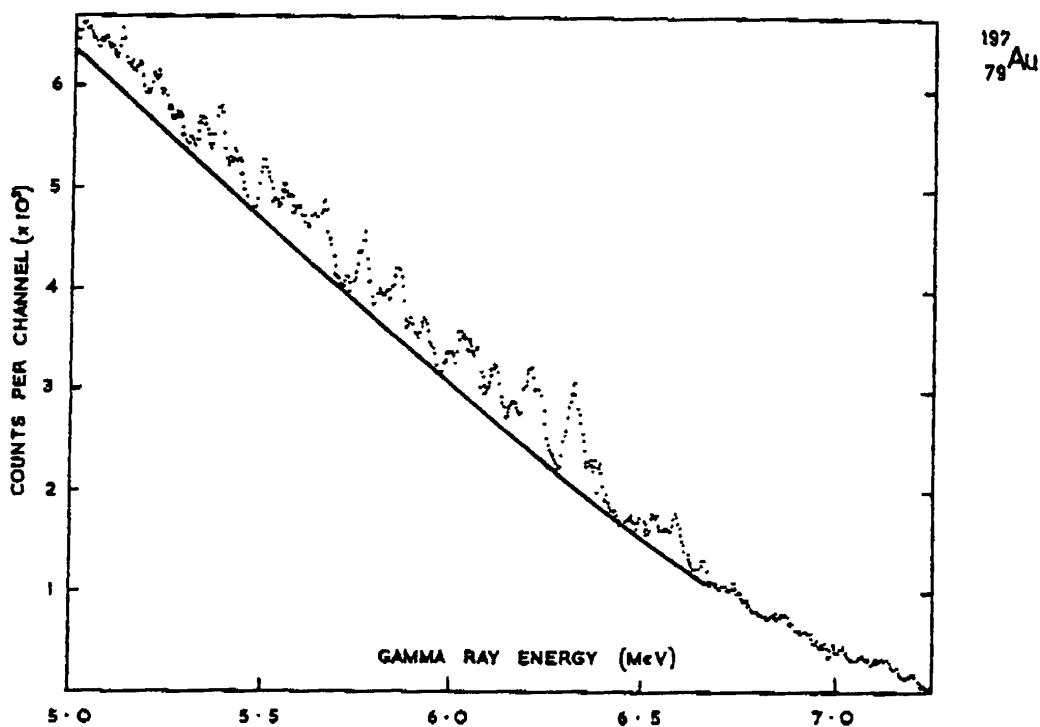


$\sigma(\theta, E_p)$. Recommended Values

Simple energy variation over large range
Nuclear Data Tables 11(1973)576

Neutron Capture in Gold

BIRD, ALLEN, BERGQVIST, AND BIGGERSTAFF



Spectrum for capture of 10 to 60 keV neutrons in gold. Target - 1.5 kg metal. Detector - Ge(Li). Escape peaks and background have been subtracted and a correction applied for neutron energy broadening of peaks (A168b). See also Be62a, F.61.

Complex energy variation in small intervall

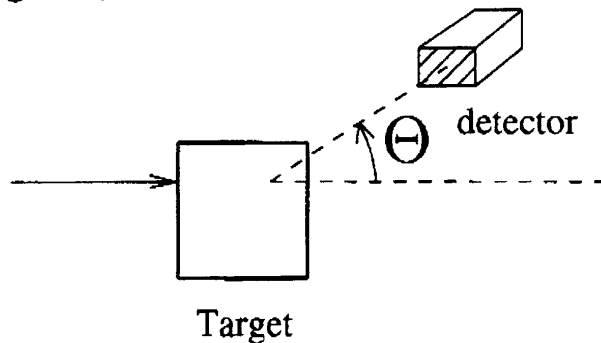
Nuclear Data Tables 11(1973)518

Neutron - Proton Scattering

$H(n,n)H$

Nuclear Physics: proton and neutron elementary particles
 \Rightarrow considered pointlike

Scattering experiment:

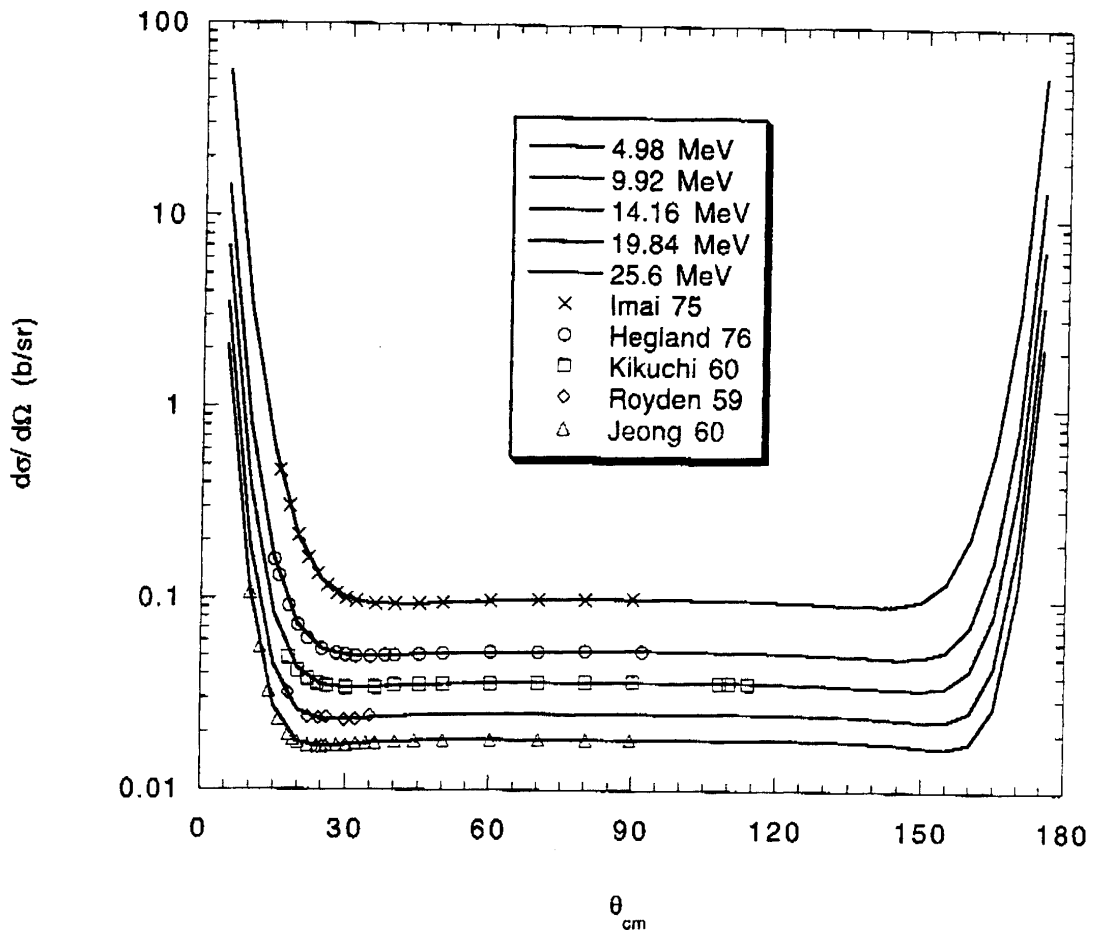


incoming neutron impinging on proton target
 $\hat{=}$ incoming wave

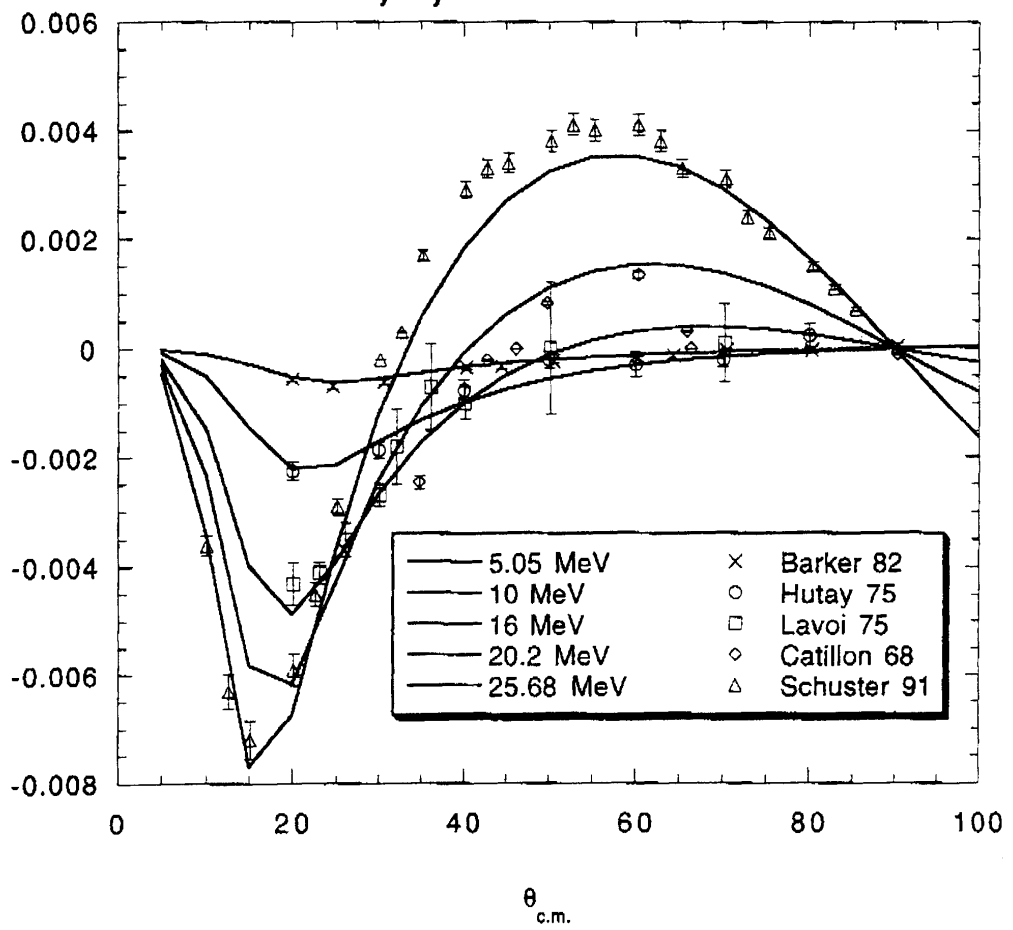
scattered neutron measured in detector
 $\hat{=}$ scattered wave

Theory: center-of-mass system
relative and center-of-mass coordinates
center-of-mass moves with constant velocity
 \Rightarrow can be separated trivially
 \Rightarrow relative motion $\hat{=}$ scattering by fixed potential

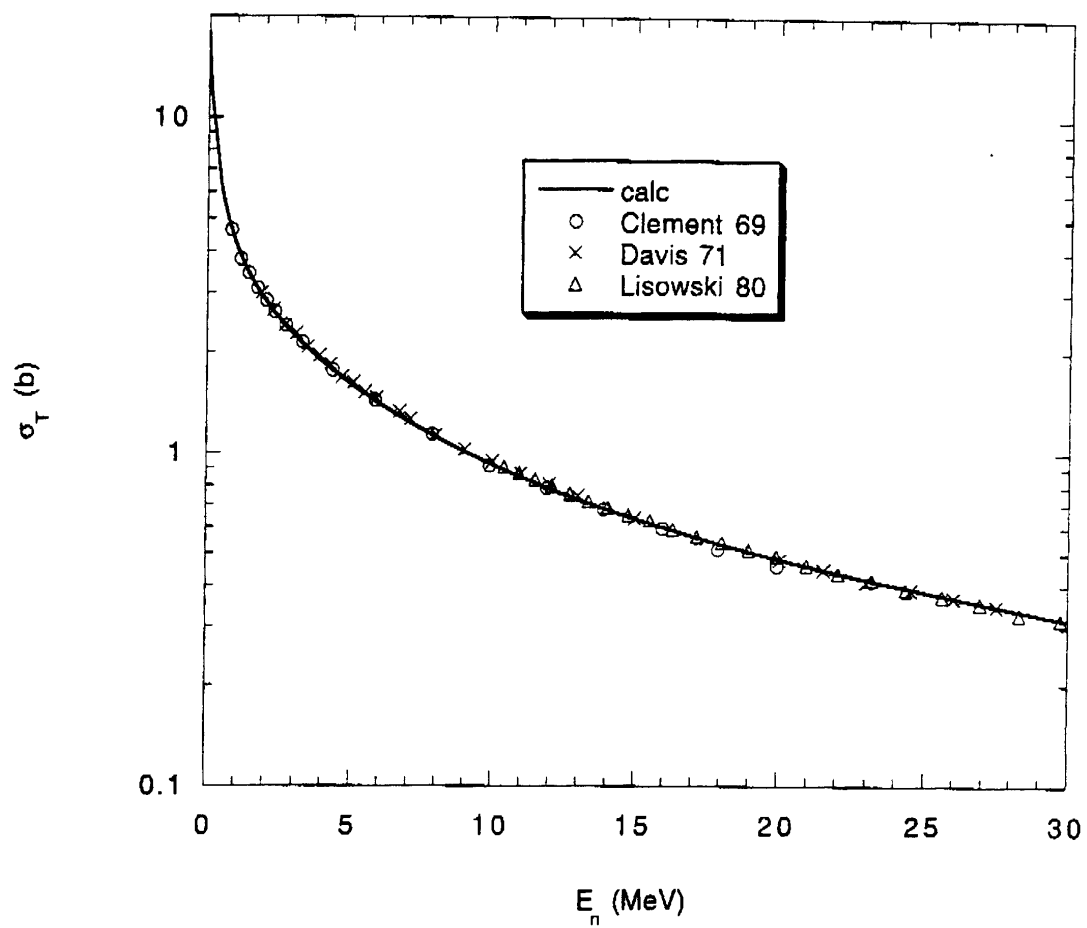
p+p Differential Cross Section



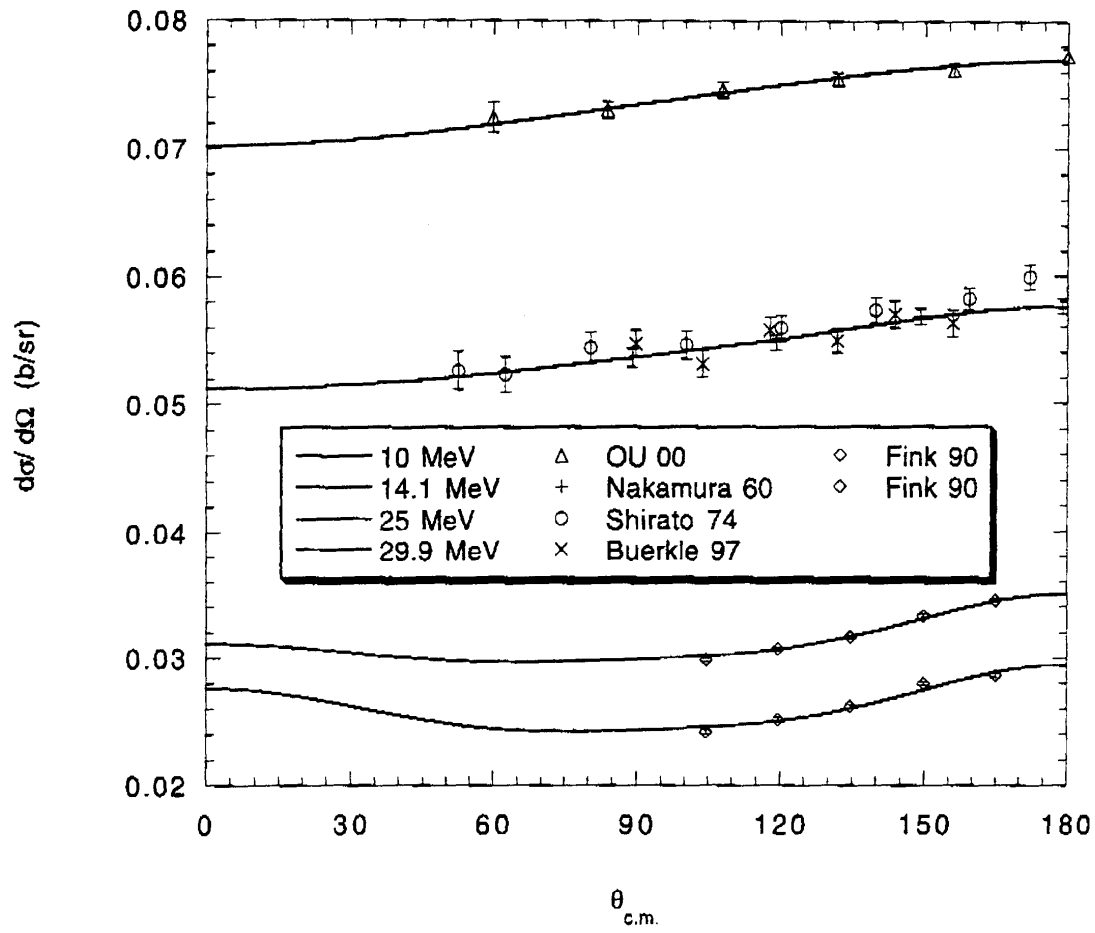
$A_y(P_y)$ for p+p Scattering



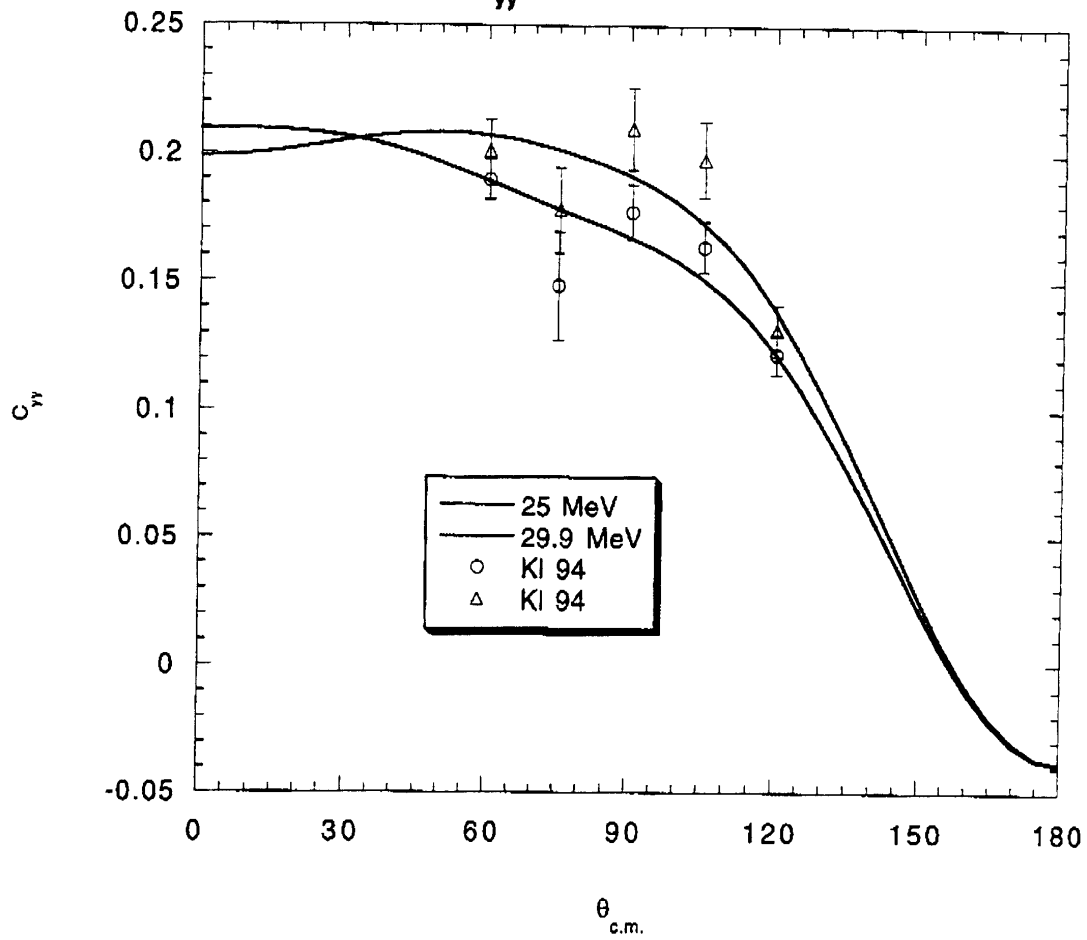
n-p Total Cross Section



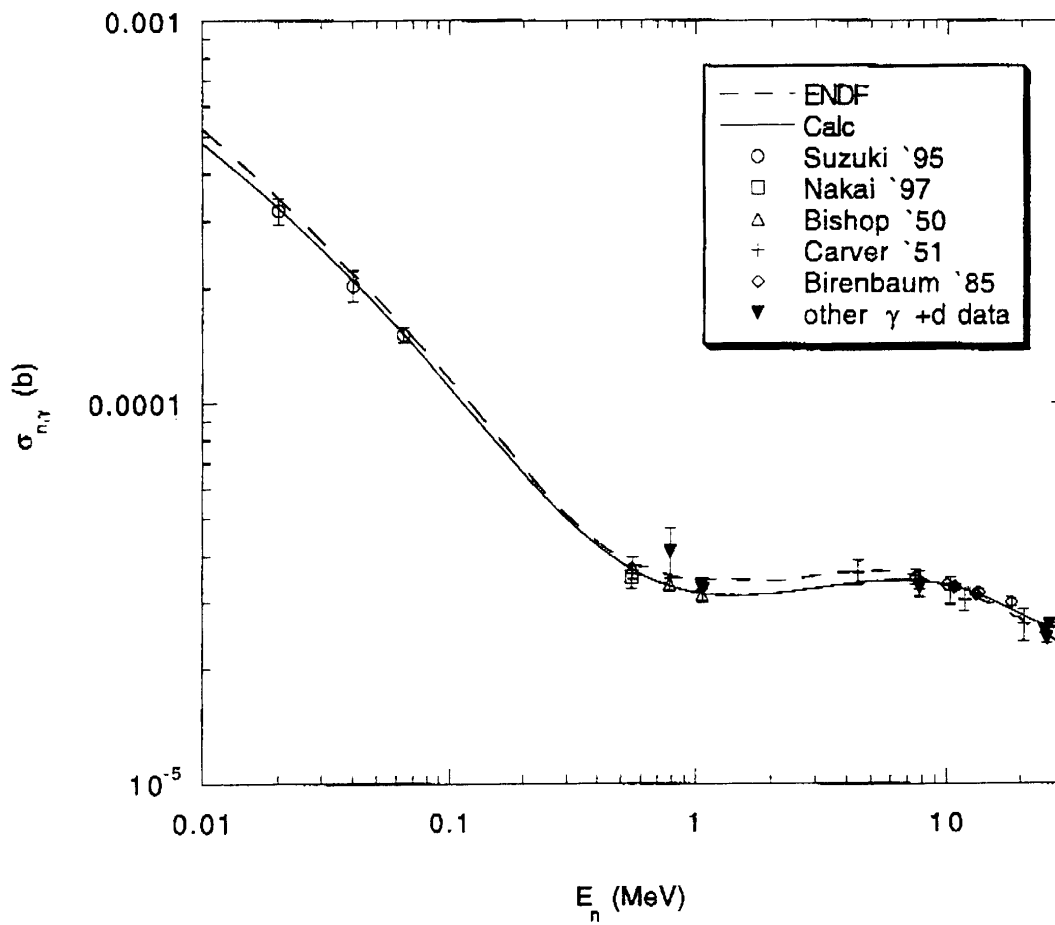
n-p Differential Cross Section



C_{yy} for n-p Scattering



n+p Capture Cross Section



Potential Scattering

Potential of finite range $\hat{=}$ interaction region

Description: Incoming free wave

modified in interaction region

scattered particles outside interaction region

free again

Dimensions: neutron beam formed far from target

dimension of beam much larger than H-atom

detector far from target

Conservation of probability:

Incoming beam

total flux through successive planes orthogonal to beam

constant

\Rightarrow Incoming beam $\hat{=}$ plane wave $\propto e^{i\vec{k}\cdot\vec{r}}$

Scattered particles

total flux through increasing spheres around potential

constant

surface of spheres \propto radius r squared

\Rightarrow Scattered particles $\hat{=}$ spherical wave $\propto \frac{e^{ikr}}{r}$

Ansatz for total wave function $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\Theta)\frac{e^{ikr}}{r}$

Differential cross section = $\frac{\text{scattered flux through area } dA}{\text{incoming flux}}$

$$d\sigma(\Theta, \phi) = |f(\Theta)|^2 d\Omega$$

Partial Wave Expansion

Potential rotationally invariant

⇒ conservation of angular momentum

⇒ angular momentum unchanged during scattering

⇒ consider each angular momentum separately

Spherical harmonics $Y_{lm}(\Theta, \phi)$ are eigenfunctions of orbital angular momentum operator

⇒ form complete set of functions for spherical angles Θ, ϕ

⇒ Any function $f(\Theta, \phi)$ can be expanded in spherical harmonics

Simplest spherical harmonic

$$Y_{00}(\Theta, \phi) = \text{const} = 1/\sqrt{4\pi}$$

Ansatz for total scattering wave function

$$\Psi(r, \Theta, \phi) = \sum_{l,m} u_l(r)/r Y_{lm}(\Theta, \phi)$$

u_l obeys radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2mE}{\hbar^2} - \frac{2mV(r)}{\hbar^2} - \frac{l(l+1)}{r^2} \right] u_l(r) = 0$$

Probability interpretation and continuity of flux
 \Rightarrow wave function u_l and derivative $du_l(r)/dr$
continuous

regular at origin: $u_l(0) = 0$

Example: No potential

$l = 0$ solutions

general solution

standing waves: $\sin kr, \cos kr$

(Riccati-)Bessel functions $j_l(kr), n_l(kr)$

In- and outgoing waves: e^{-ikr}, e^{ikr}

Hankel functions $h_l^{(1)}(kr), h_l^{(2)}(kr)$

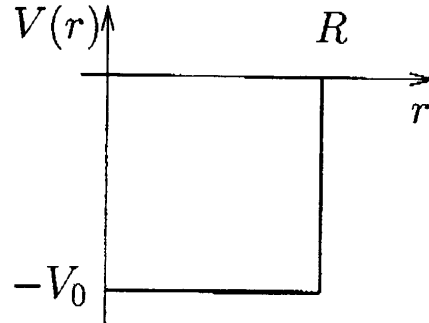
regularity \Rightarrow only $\sin kr$ allowed

Scattering Phase Shift

Example:

square-well potential, $\ell = 0$

$$V(r) = \begin{cases} -V_0 & r \leq R \\ 0 & r > R \end{cases}$$

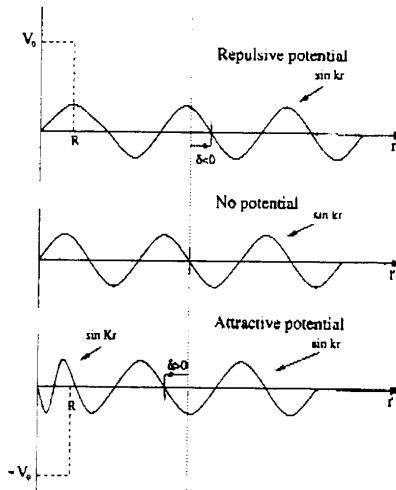


wave function

$$u_0(r) = \begin{cases} \sin Kr & r \leq R \\ A \sin kr + B \cos kr & r > R \\ \propto \sin(kr + \delta_0) \end{cases}$$

with $k^2 = 2mE/\hbar^2$ and $K^2 = 2m(E + V_0)/\hbar^2$
for $r = R$ logarithmic derivative of u_0 continuous

$$\Rightarrow \tan \delta_0 = B/A$$



\Rightarrow weak potential: attractive $\delta > 0$

repulsive $\delta < 0$

phase shift δ is function of energy

S-Wave Scattering

No potential

$$\psi_0 = \frac{\sin kr}{kr} = \underbrace{\frac{1}{2ikr}}_{\text{outgoing}} (e^{ikr} - \underbrace{e^{-ikr}}_{\text{incoming wave}})$$

with potential, outside potential

$$\psi_0 = N \frac{\sin(kr + \delta_0)}{kr} = \frac{1}{2ikr} (S_0 e^{ikr} - e^{-ikr})$$

outgoing wave is modified, incoming must not

$$\psi_0 = \frac{N}{2ikr} (e^{ikr + i\delta_0} - e^{-ikr - i\delta_0})$$

$$\Rightarrow N = e^{i\delta_0} \quad \text{and} \quad S_0 = e^{2i\delta_0}$$

$$\psi_0 = \frac{e^{i\delta_0}}{2ikr} (e^{ikr + i\delta_0} - e^{-ikr - i\delta_0})$$

$$= \underbrace{\frac{1}{2ikr} (e^{ikr} - e^{-ikr})}_{\text{free wave}} + \underbrace{\frac{e^{ikr}}{2ikr} (e^{2i\delta_0} - 1)}_{\text{scattered wave } \psi_{sc}}$$

$$\psi_{sc} = \frac{e^{ikr}}{kr} e^{i\delta_0} \sin \delta_0 = \frac{e^{ikr}}{r} f_{l=0}(\Theta)$$

$$\text{Partial cross section: } \frac{d\sigma}{d\Omega} = |f_{l=0}(\Theta)|^2 = \frac{\sin^2 \delta_0}{k^2}$$

Energy Dependence of Scattering Phase Shifts

Physical quantities contain phase shifts only in expressions like $e^{2i\delta}$ or $e^{i\delta} \sin \delta$

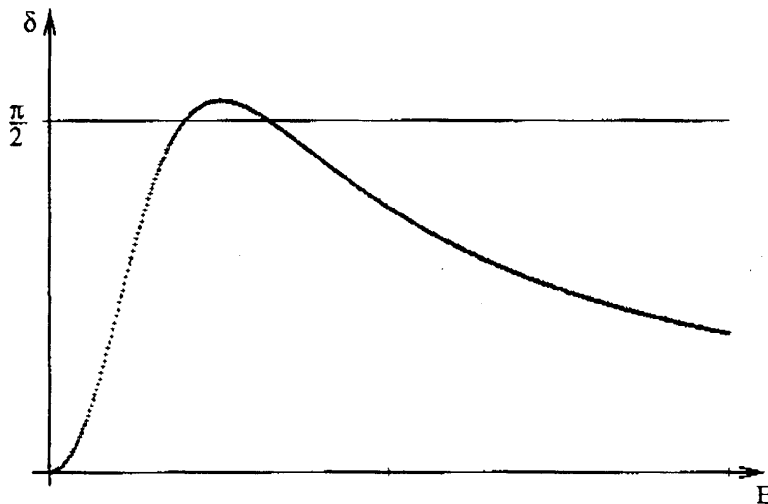
\Rightarrow multiples of π do not matter for δ

Standard choice $\delta(Energy = \infty) = 0$

Levinson theorem:

$\delta(E = 0) - \delta(E = \infty) = \text{number of bound states} \times \pi$

Typical behaviour



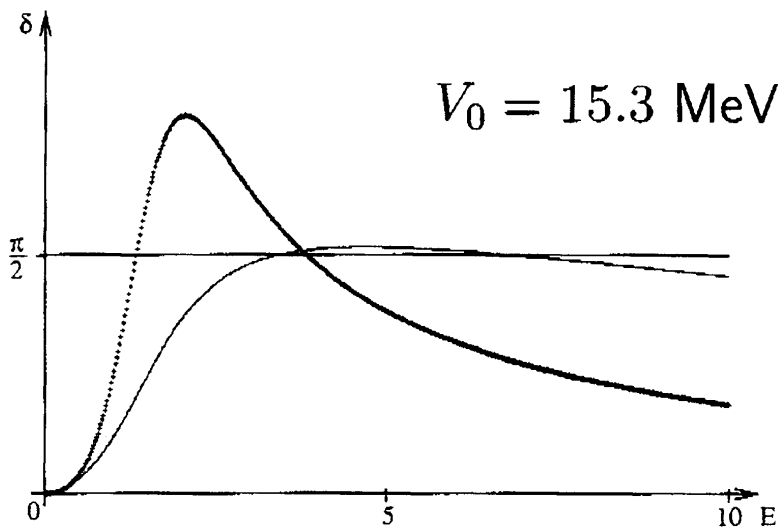
Example: P-Wave Phase Shifts

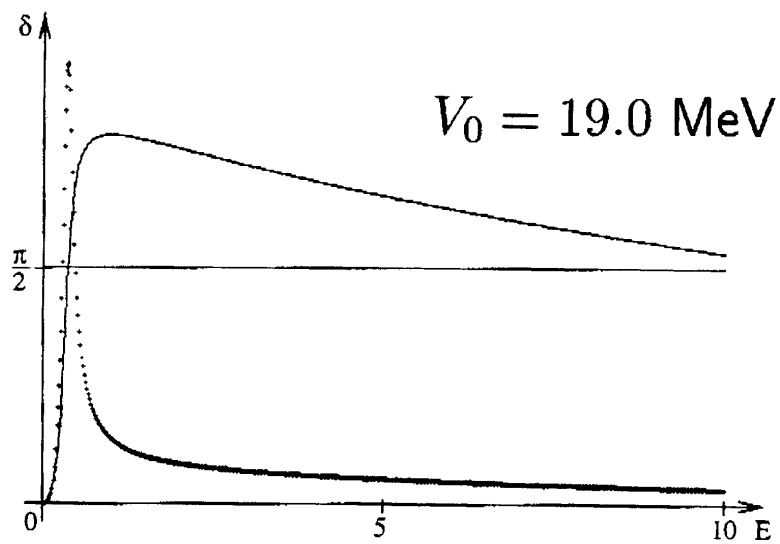
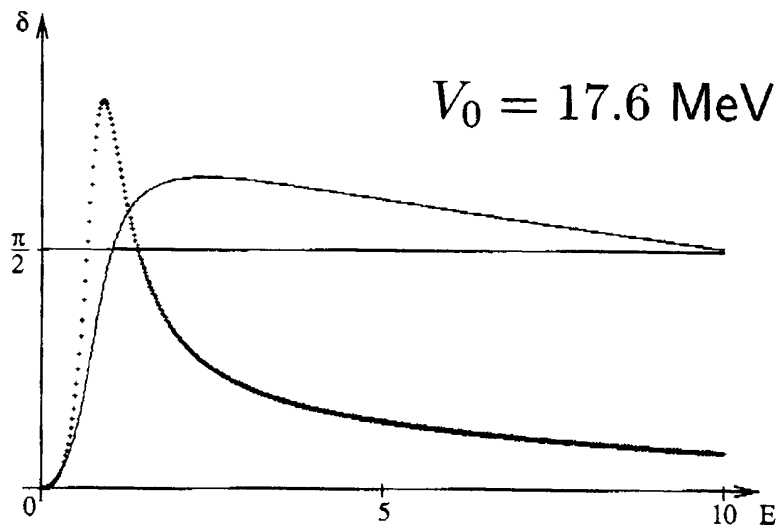
Exercise:

Spherical square well potential, range $R = 3.14\text{fm}$

energy range considered 0 - 14 MeV

plot $\delta_{l=1}$ and $\sigma_1 = 4\pi^3 \sin^2 \delta / k^2$ as function of energy for $V_0 = 15.3, 17.6,$ and 19.0 MeV
($M = 1000 \text{ MeV}/c^2, \hbar c \approx 200 \text{ MeV fm}$) $j_1(4.49) \approx 0$





Note: Only narrow resonances have their maximum at $\delta = \frac{\pi}{2}$

Neutron - Proton - Scattering

Nuclear Physics: neutron and proton elementary particles

What do we know about their interaction ?

$n + p$ form bound state deuteron $J^\pi = 1^+$

no $n + n$, or $p + p$ bound state known

$n + p$ state with spin zero unbound

⇒ NN interaction spin-isospin dependent

Simplest deuteron model: attractive potential, spin $S = 1$, no orbital angular momentum

However, deuteron has quadrupole moment

⇒ aspherical shape needed

⇒ need higher orbital angular momenta of positive parity

⇒ D -wave component $\ell = 2$, coupled channels

S - wave: $(l = 0, S = 1)^{J=1^+}$

D - wave: $(l = 2, S = 1)^{J=1^+}$

⇒ need non-central tensor force

General Nucleon-Nucleon Force

$$V_{NN}(\vec{r}) = V_{central}(r)$$

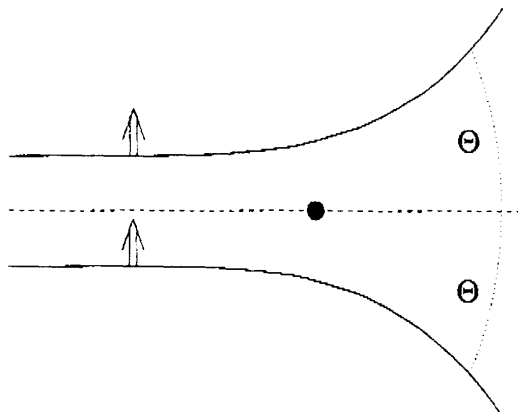
no direction distinguished, can be different for parallel spins $\uparrow\uparrow$ and anti-parallel spins $\uparrow\downarrow$

$$+ V_{tensor}(r) \left[Y_2(\hat{r}) [\vec{\sigma}_1 \vec{\sigma}_2]^2 \right]^0 \text{ spins parallel } \uparrow\uparrow$$

$$\propto \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2 - \frac{1}{3} r^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$+ V_{spin-orbit}(r) \vec{L} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$$

distinguishes left-right scattering of polarized nucleons



Observable: polarization (measured in exit channel)

analysing power (prepared in initial channel)

measures interference of different partial waves

\Rightarrow sensitive to small components

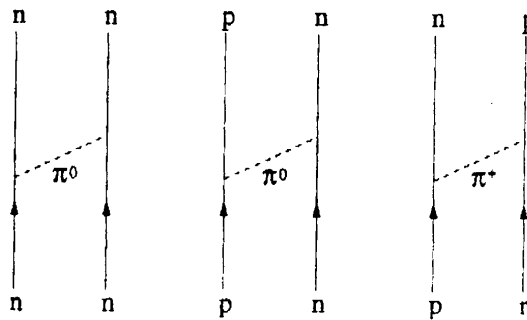
Theoretical Approach

Quantum - Chromo - Dynamics: THE theory of strong interactions also governs nuclear physics
However, no solutions known till now

Instead of QCD degrees of freedom, quarks and gluons, use hadron degrees, nucleons and mesons

Meson-Exchange-Models

long range part dominated by lightest meson, the pion
Model parameters fitted to deuteron properties and many scattering data



radial dependence of short range phenomenologic

⇒ Paris-, Argonne-, Nijmegen- ... potential

radial dependence of short range given by heavy mesons

⇒ Bonn-, Moscow-, ... potential

These potentials, so called realistic

NN-potentials, reproduce pp and np data within error bars, due to fit

See following figures for NN-data

Idea: use these potentials to describe reactions of heavier nuclei

S-Wave Scattering

No potential

$$\psi_0 = \frac{\sin kr}{kr} = \underbrace{\frac{1}{2ikr}}_{\text{outgoing}} (e^{ikr} - \underbrace{e^{-ikr}}_{\text{incoming wave}})$$

with potential, outside potential

$$\psi_0 = N \frac{\sin(kr + \delta_0)}{kr} = \frac{1}{2ikr} (S_0 e^{ikr} - e^{-ikr})$$

outgoing wave is modified, incoming must not

$$\Rightarrow N = e^{i\delta_0} \quad \text{and} \quad S_0 = e^{2i\delta_0}$$

$$\begin{aligned} \psi_0 &= \frac{e^{i\delta_0}}{2ikr} (e^{ikr+i\delta_0} - e^{-ikr-i\delta_0}) \\ &= \underbrace{\frac{1}{2ikr} (e^{ikr} - e^{-ikr})}_{\text{free wave}} + \underbrace{\frac{e^{ikr}}{2ikr} (e^{2i\delta_0} - 1)}_{\text{scattered wave } \psi_{sc}} \end{aligned}$$

$$\psi_{sc} = \frac{e^{ikr}}{kr} e^{i\delta_0} \sin \delta_0 = \frac{e^{ikr}}{r} f_{l=0}(\Theta)$$

$$\text{Partial cross section: } \frac{d\sigma}{d\Omega} = |f_{l=0}(\Theta)|^2 = \frac{\sin^2 \delta_0}{k^2}$$

R-Matrix Data Analysis

Idea: Separate configuration space in two parts

I: Interaction region of finite channel radius a

II: asymptotic space (no interaction, except point Coulomb)

Solution in II known, free incoming and outgoing waves, $I - S(E)O$

Hamiltonian not hermitian in finite space

Choose boundary condition B, derivative zero

Instead $(H - E)u_E = 0$ use

$$(H + \mathcal{L}_B - E)u_E = \mathcal{L}_B u_E$$

$$u_E = \underbrace{(H + \mathcal{L}_B - E)^{-1}}_{\text{Blacksfunction } G} \mathcal{L}_B u_E$$

Eigenfunctions of H in I u_λ form complete set

expand in I G and u_E in terms of u_λ

$$\Rightarrow u_E(r) = G(r, a) a \frac{du_E}{dr} \Big|_a \text{ and}$$

$$G(r, a) \propto \sum_\lambda \frac{u_\lambda(r) u_\lambda(a)}{E_\lambda - E}$$

Define R-Matrix

$$R = \frac{u_E(a)}{a \frac{du_E}{dr} \Big|_a} = G(a, a) = \sum_\lambda \gamma_\lambda^2 / (E_\lambda - E)$$

Connection to Scattering Matrix

In asymptotic region II $u_E \propto I - S(E)O$
 logarithmic derivative continuous at channel
 radius a

$$R = \underbrace{\frac{u_E}{au'_E}}_{\text{internal}} \Big|_a = \underbrace{\frac{I - SO}{a(I' - SO')}}_{\text{asymptotic}} \Big|_a$$

$$\Rightarrow S(E) = \frac{I(a)}{O(a)} \frac{1 - L_I R}{1 - L_O R}$$

with $L_O = \frac{aO'(a)}{O(a)} = \left(\frac{aI'(a)}{I(a)} \right)^* = (L_I)^*$

In simple case: L_O positive imaginary

\Rightarrow poles of S in lower half-plane

Data analysis:

Use finite number of R-matrix pole positions
 (energies E_λ) and residues (reduced width
 amplitudes γ_λ) to reproduce data

Physical Constraints in R-Matrix Theory

Unitarity ($SS^\dagger = S^\dagger S = \mathbf{1}$)

comes from R real (hermitian), constraints
S-matrix elements for different reactions

Built-In Symmetries of Strong Interaction

Conservation of angular momentum and parity

Time - reversal invariance due to R, S symmetric

Approximate Symmetry

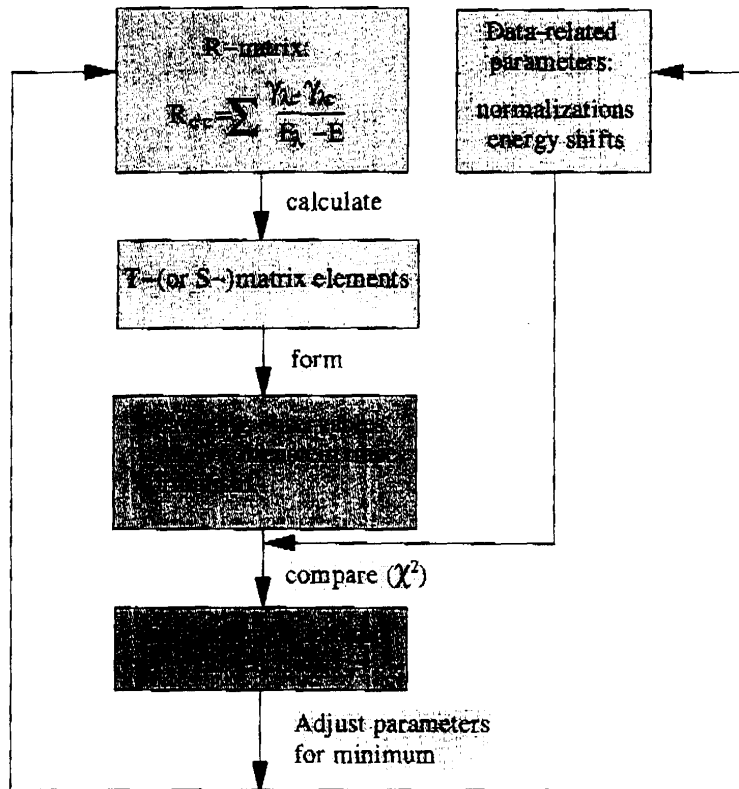
Charge independence (charge symmetric)

Truncation of nuclear partial wave series

Due to finite channel radius and

Coulomb/angular-momentum barrier

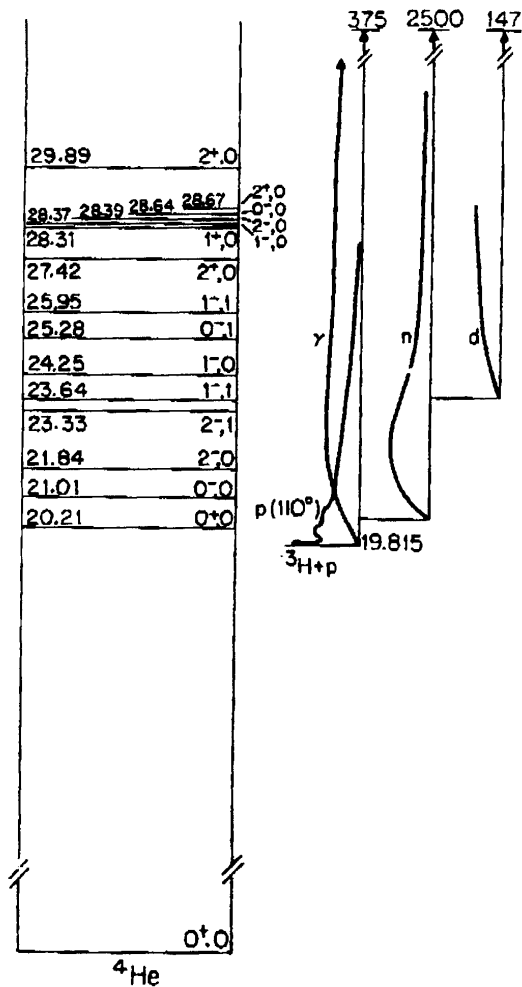
Energy Dependent Analysis Code



Capabilities and Features

- 1) Accommodates general (spins, masses, charges) two-body channels
- 2) Uses relativistic kinematics and R-matrix formulation
- 3) Calculates general scattering observables for $2 \rightarrow 2$ processes
- 4) Has rather general data-handling capabilities
- 5) Uses modified variable-metric search algorithm that gives parameter covariances at a solution.

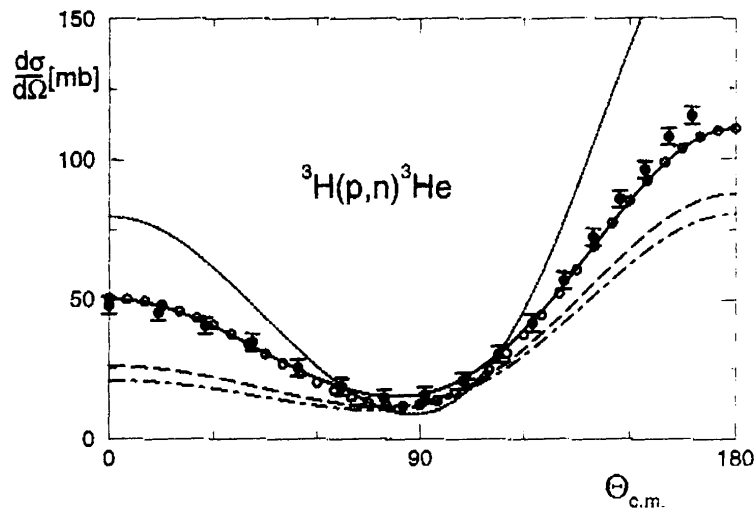
^4He Level Scheme



physical channels: proton - triton, neutron - ^3He ,
 deuteron - deuteron
 several channel spins possible
 \Rightarrow coupled channels

The Reaction ${}^3\text{He}(n, p)t$

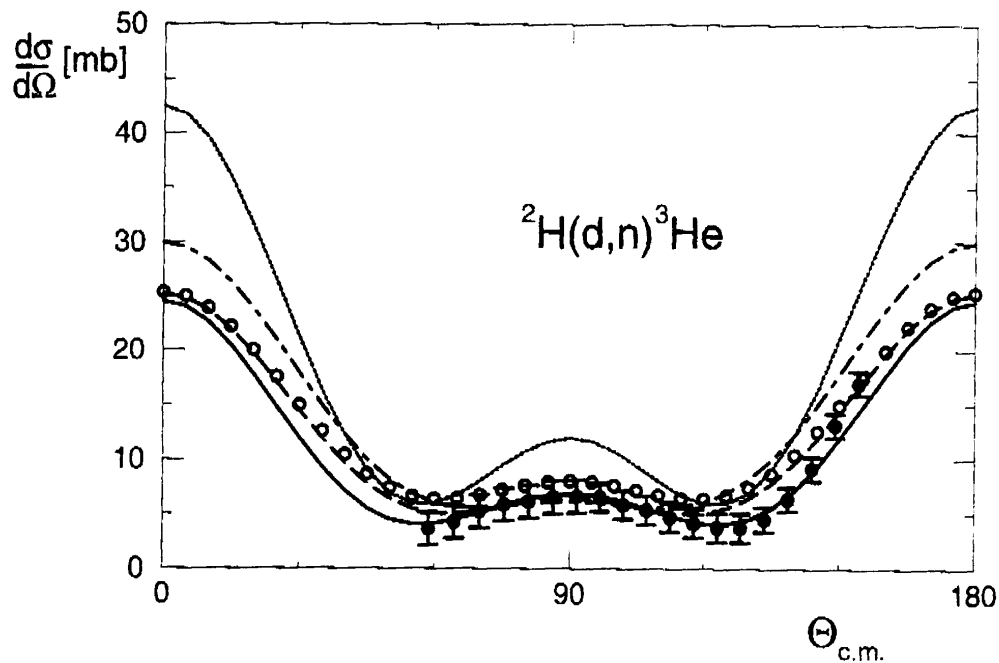
Due to open channels always coupled channels
Four-body problem, difficult to calculate
huge computer power necessary
only qualitative agreement with data
bit prior information into R-matrix analysis
many parameters necessary
e.g. $\ell = 2$: 36 channels; $\ell = 3$: 51 channels



Differential cross section of the reaction ${}^3\text{H}(p, n){}^3\text{He}$ calculated for $E_{cm} = 3.0$ MeV. The data are for 4.101 MeV protons from Perry. The full line represents the R -matrix analysis, the dashed one the full calculation, the dot-dashed one the small calculation, and the dotted one the semi-realistic calculation. The open circles denote the full calculation with the 3P_2 matrix element replaced by the corresponding R -matrix one.

Difficulties of Analysis

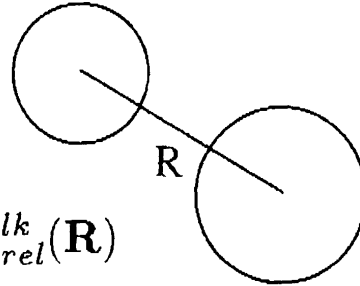
- Many coupled channels \Rightarrow many parameters
- Resonances very broad \Rightarrow not too well defined
- background problematic
- not enough data
- inconsistent data
- How to treat break-up channels



Differential cross section for the reaction ${}^2\text{H}(d,n){}^3\text{He}$ calculated for $E_{cm} = 2.11$ MeV. Data are for 4.0 MeV deuterons from Schulte. The labeling is as before.

Resonating Group Model Ideas

Composite system



$$\text{RGM Ansatz } \Psi_l = \sum_{k=1}^{chan} \psi_{chan}^k \cdot \chi_{rel}^{lk}(\mathbf{R})$$

$$\text{Variation } \langle \delta \Psi_l | \mathcal{A} | H - E | \Psi_l \rangle = 0$$

$$\text{Channel function } \psi_{chan} = [Y_L(\hat{\mathbf{R}}) \otimes [\phi_1^{j_1} \otimes \phi_2^{j_2}]^{S_c}]^J$$

$$\text{Ansatz } \psi = \psi_{chan}(\sum_i b_i \cdot \text{Gaussian}) \quad (\text{bound state})$$

$$\text{or } \chi_{rel}^{lk}(R) = \delta_{lk} \cdot F_k(R) + a_{lk} \cdot \tilde{G}_k(R) + \sum_i b_{lki} \cdot \text{Gaussian} \\ (\text{scattering state})$$

Variational parameters a_{lk} and $b_{(lk)i}$

Decompose Hamiltonian

$$\begin{aligned} H - E &= H_1 - E_1 + H_2 - E_2 + \\ &\sum_{\substack{i \in 1 \\ j \in 2}} V_{ij} - V_{Coul} + \\ T_R + V_{Coul} - (E - E_1 - E_2) &= \\ H_1 - E_1 + H_2 - E_2 + V_{short} + H_R - \tilde{E} \end{aligned}$$

$$\text{with } \mathcal{A} \cdot (H_i - E_i) \phi_i = 0 \text{ and } (H_R - \tilde{E}) F/G = 0$$

\Rightarrow All integrals shortranged

Note: Relative thresholds fixed by \tilde{E}

Resonating Group Model Technicalities

⇒ Expand all Functions including F and G

- in terms of Gaussians
- times solid spherical harmonics
- times monomials in R^2

⇒ All individual integrals analytically calculable,
provided potential is of Gaussian form including differential operators
All Operators allowed which occur in Argonne and Bonn (r-space)
potentials

- Correct center of mass motion
- No limit on number of channels
- No limit on number of nucleons
- Up to 6 clusters, i.e. up to 6 orbital angular momenta

⇒ Allow for distortion of fragments via different ϕ and/or
different decompositions of the system

Three- and more-body channels approximately treated via two-body
channels

Fragment wave functions ϕ_1 and ϕ_2 must be strongest bound in given
model-space

⇒ Relative thresholds can only be changed by increasing dimension of
model-space or other potential

Effective Interactions versus Realistic ones

Effective interactions

- simple wave functions
- comparatively fast calculations, e. g. ^{10}B - neutron scattering
- parameter studies possible
- model space dependence unclear
- severe overbinding possible
- limited energy range, $E_{\text{threshold}} + \approx 25 \text{ MeV}$

Realistic interactions

- complicated wave functions
- tedious long lasting calculations
- model spaces increase rapidly with A , limit around $A = 6$
- parameterfree calculation
- calculation improves with increasing model space
- no overbinding possible
- large energy range, up to pion threshold

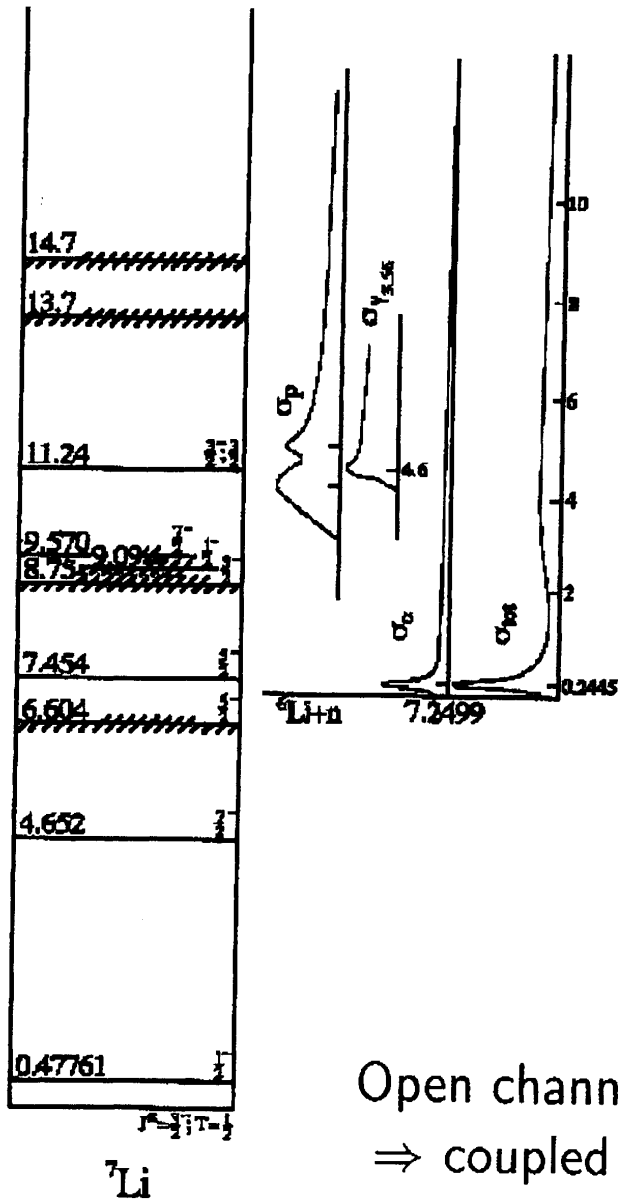
Strategy

Study small system A

Blackuce model space till qualitative change

Use this model space as input for $A + 1$ system

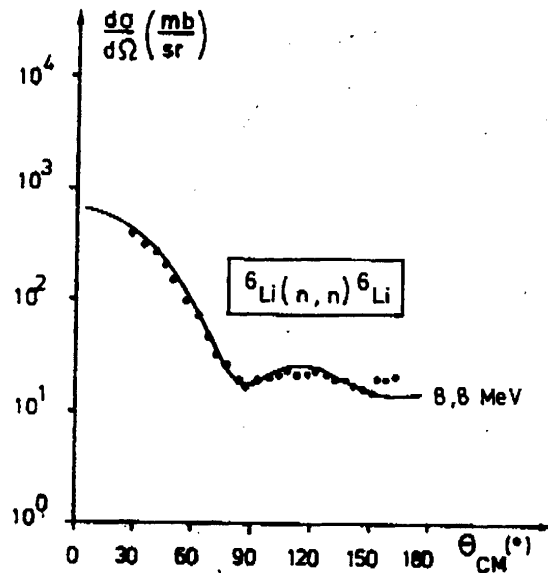
${}^6\text{Li}(n, t)\alpha$ Reaction



Open channel α - triton
 \Rightarrow coupled channels

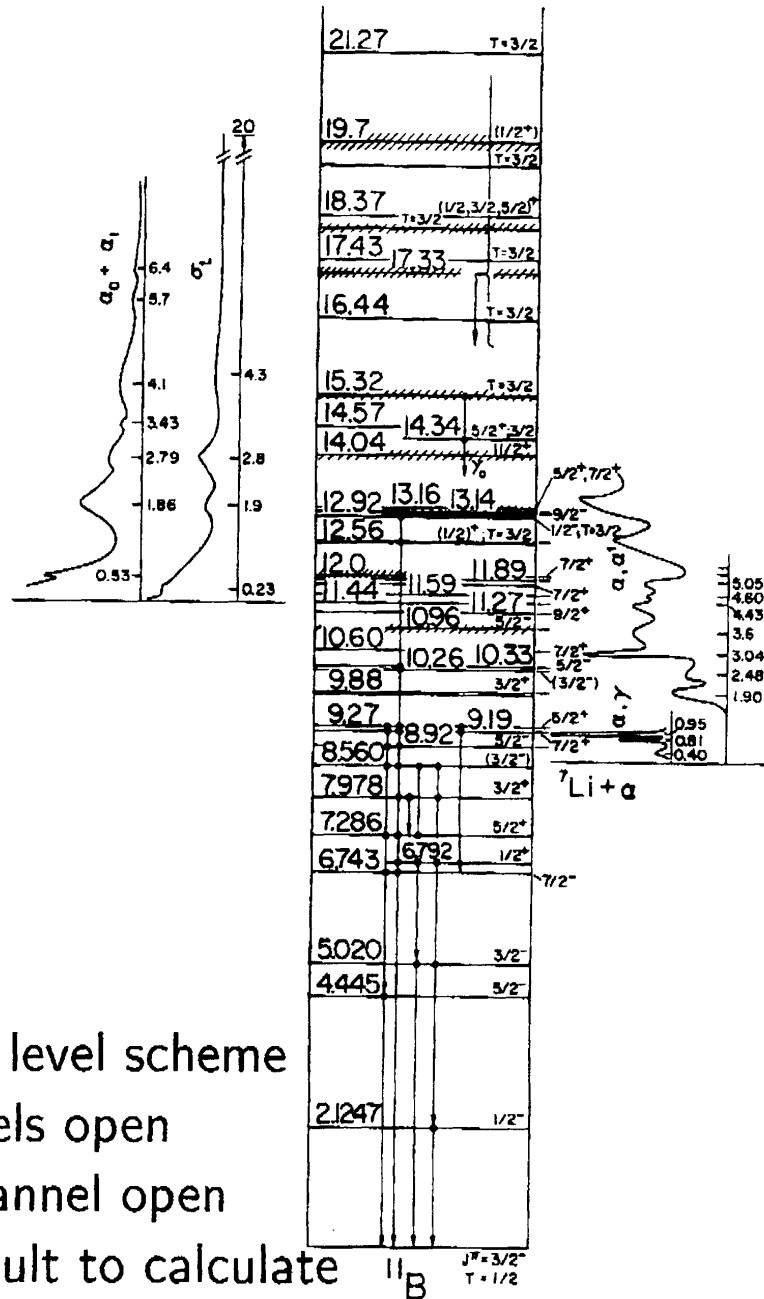
Well defined, narrow $\frac{5}{2}^-$ resonance in relevant energy range

Typical Resonating Group Result



M. Herman 1985 unpublished
see also 'Use of the Optical Model for ...
Neutron Cross-Sections ...', NEADC-222 'U'
page 77, OECD Paris 1986

$^{10}\text{B}(n,\alpha)^7\text{Li}$ Reaction



Complicated level scheme
 Many channels open
 Break-up channel open
 \Rightarrow very difficult to calculate
 Data analysis tedious

General Nucleon-Nucleon Force

$$V_{NN}(\vec{r}) = V_{central}(r)$$

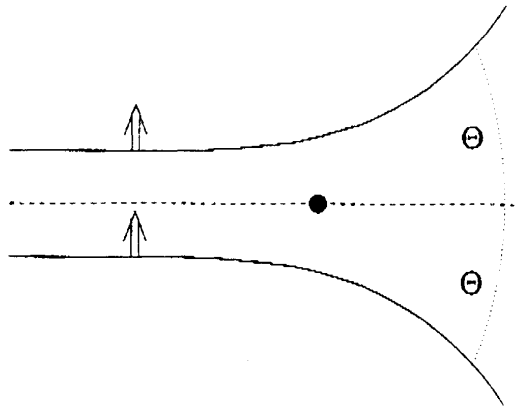
no direction distinguished, can be different for parallel spins $\uparrow\uparrow$ and anti-parallel spins $\uparrow\downarrow$

$$+ V_{tensor}(r) \left[Y_2(\hat{r}) [\vec{\sigma}_1 \vec{\sigma}_2]^2 \right]^0 \text{ spins parallel } \uparrow\uparrow$$

$$\propto \vec{r} \cdot \vec{\sigma}_1 \vec{r} \cdot \vec{\sigma}_2 - \frac{1}{3} r^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

$$+ V_{spin-orbit}(r) \vec{L} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$$

distinguishes left-right scattering of polarized nucleons



Observable: polarization (measured in exit channel)

analysing power (prepared in initial channel)

measures interference of different partial waves

\Rightarrow sensitive to small components