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WORKSHOP ON NUCLEAR MODEL COMPUTER CODES

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SPHERICAL OPTICAL MODEL OF NUCLEAR REACTIONS

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Programme

1. Introduction
   - Evaluation procedure
   - Place of the SOM and CCM

2. The optical model
   - Definition
   - The corresponding Schroedinger equation
   - The different potentials
   - Usual values of the parameters

3. The numerical solution
   - Matching radius
   - The external region
   - The internal region
   - Matching
   - Output quantities

4. The program SCAT2
   - Presentation
   - Input data description
   - Test case

5. Proposed exercises
   - Sensivity to the parameters
   - n + 56-Fe
   - Miscellaneous.

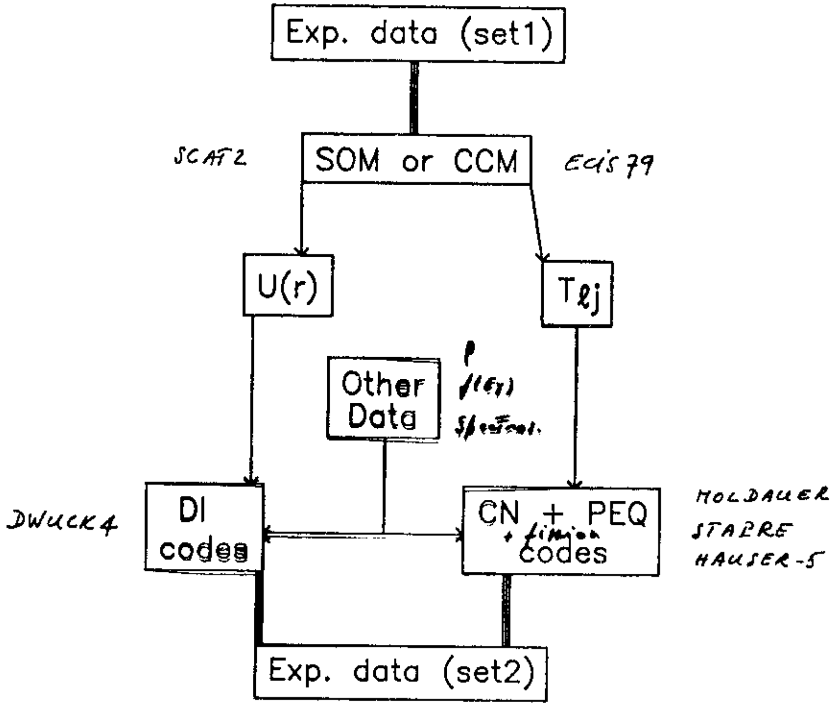
• not a theoretical lecture about SOM (text books)
  but the user's point of view

• experimentation → interpretation — n + A system
  create data file – complete: σ, $\frac{d\sigma}{d\Omega}$, $\frac{d\sigma}{dE}$, …
  – partial
  Evaluation (consistent)

• ignore the resonance region

• – compound nucleus
  – direct process

• provide an evaluation starting from
  – exp. data (may be insufficient, incoherent, sparse, …)
  – models (codes)
    . results are coherent (Σ of partials)
    . interpolate, extrapolate data
    . need exp. data to adjust some param.
  [illegible]



G. REFFO

Evaluation procedure

- feed backs

- SOM

- Exp. or general theory of N reactions → fluctuating cross sections

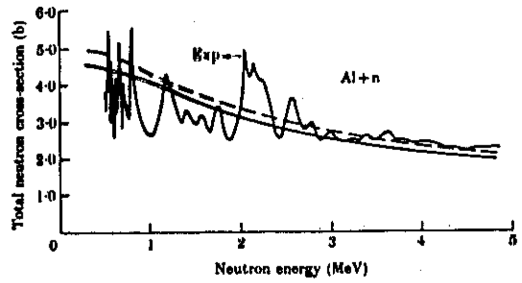


FIG. 5.6. Measured total neutron cross-sections for ^{27}Al compared with optical-model calculations with parameters fitted to energy-averaged cross-sections. (E. Auerbach and S. O. Moore, *Phys. Rev.* 163, 1124, 1967.)

- Simplification: define potentials to reproduce the slowly varying cross section (average)

- The potential for the elastic scattering is the optical model potential
  - ~ same spatial expansion as the nucleus

- Restrictions: – E large (many states → average)
  - elastic channel not strongly coupled to any non-elastic channel (CCM)

- Basic eqn: $\left[-\frac{\hbar^2}{2\mu}\nabla^2 + U(r) - E\right]\Phi(\vec{r}_1,\vec{r}_2) = 0$

  to be solved.

- Physical equation [illegible]
- Centre of mass system $f(\vec{r}_1, \vec{r}_2) = f(\vec{R})\, \varphi(\vec{r})$
- Simplifications: V short range, contact $V(\vec{r}, \vec{r}\,') = V(r)\, \delta(\vec{r} - \vec{r}\,')$
  - of Ψ_{in} $\Psi(\vec{r}) = \exp(i\vec{k}\cdot\vec{r}) = \exp(ikz)$
  - of Ψ_{sc} as asymptotic form (r large)
    $\Psi(\vec{r}) = e^{ikz} + f(\theta)\, \frac{e^{ikr}}{r}$

- Spherical coordinates: – separation of variables r, θ, φ
  – partial waves decomposition

$$\Psi(\vec{r}) = \frac{4\pi}{kr} \sum_{\ell=0}^{\infty} i^\ell u_\ell(r)\, \frac{(2\ell+1)}{4\pi}\, P_\ell(\cos\theta)$$

where u_ℓ is solution of the radial eqn

$$\Rightarrow \left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2}\, U(r) - \frac{\ell(\ell+1)}{r^2} \right] u_\ell(r) = 0$$

- if $U(r) = 0$ Ψ_{inc}
- if $U(r) \neq 0$ $\Psi_{tot} = \Psi_{inc} + \Psi_{sc}$
  $\hookrightarrow f(\theta)$ and σ by flux considerations

Optical potential

5 terms: $U(r) =$

$V_C(r)$	Coulomb
$-\ V\ f(r)$	real (volume)
$+\ i\ W_S\, g(r)$	imaginary surface
$-\ i\ W_V\, f(r)$	imaginary volume
$+\ C_{SO}(\vec{l}\cdot\vec{s})\ V_{SO}\ h(r)$	spin-orbit (elastic)

[illegible]

f, g, h = form factors

$\lim_{r\to\infty} r\, U(r) = 0$, not satisfied for Coulomb potential.

Volume WOODS-SAXON

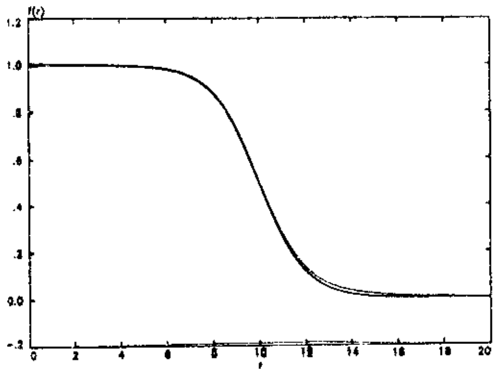
$$f(r) = \frac{1}{1+X} \qquad X = \exp\frac{r-R_1}{a_1} \qquad R_1 = r_1 A^{1/3}$$

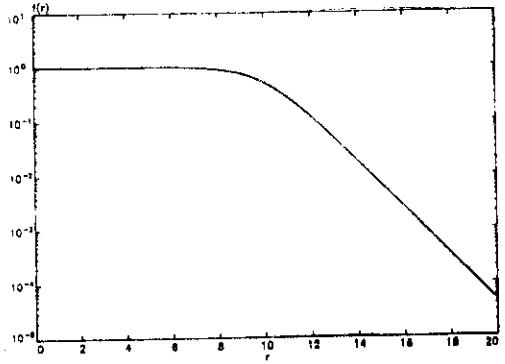
$$f'(r) = -\frac{1}{a_1}\frac{X}{(1+X)^2} \qquad f(R_1) = 1/2$$

$$f'(R_1) = -\frac{1}{4a_1}$$

$$f''(r) = -\frac{1}{a_1^2}\frac{X(1-X)}{(1+X)^3} \qquad f''(R_1) = 0$$

Example: $R_1 = 10$, $a_1 = 1$ fm





$$f(r_m) = \frac{1}{\alpha} \quad \text{for } r_m = R_1 + a_1 \log(\alpha - 1)$$

α	r_m
10	$R_1 + 2.2\,a_1$
100	$R_1 + 4.6\,a_1$
100	$R_1 + 6.9\,a_1$

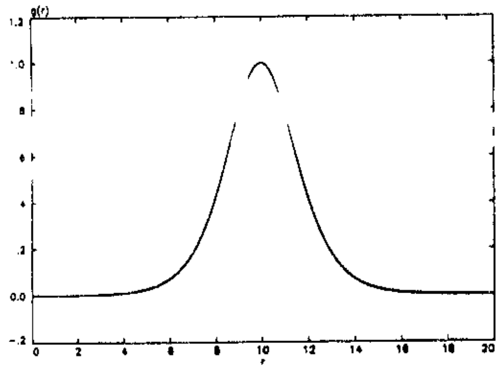
Practical calculation: $\exp\frac{nh - R_1}{a_1} = \left[\exp\frac{h}{a_1}\right]^n \exp\left(-\frac{R_1}{a_1}\right)$

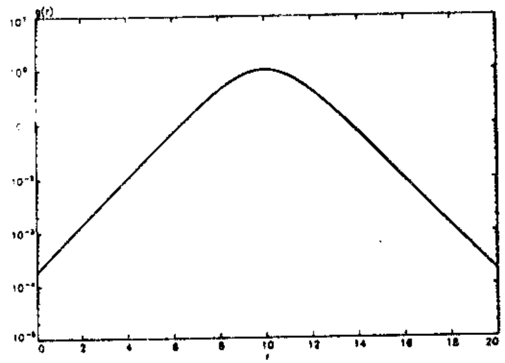
Surface: Derivative WOODS-SAXON (DWS)

$$g(r) = -4a_2\frac{df}{dr} = 4\frac{X}{(1+X)^2} \qquad X = \exp\frac{r-R_2}{a_2} \qquad R_2 = r_2 A^{1/3}$$

$$g(R_2) = 1, \qquad g(r) = 1/2 \quad \text{for } r = R_2 + a_2 \log(3 \pm 2\sqrt{2})$$

Example: $R_2 = 10$, $a_2 = 1$ fm.





$$g(r_m) = \frac{1}{\alpha} \quad \text{for } r_m = R_2 + a_2 \log\left(2\alpha - 1 \pm \sqrt{4\alpha(\alpha-1)}\right)$$

α	r_m
10	$R_2 + 3.6\,a_2$
100	$R_2 + 6.0\,a_2$
1 000	$R_2 + 9.3\,a_2$

Practical calculation: as $f(r)$.

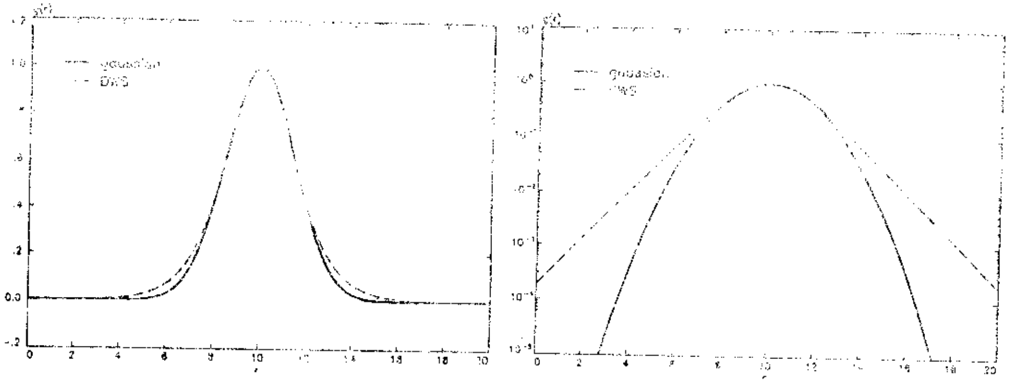
$g(R_0) = \frac{1}{2}$, $g(r_g) = \frac{1}{e}$ for $r_g = R_0 \pm a_g$

gaussian with same fwhm as DWS

$R' = R$, $a' = \frac{a}{\sqrt{\log 2}} \log\left(\frac{3+2\sqrt{2}}{3-2\sqrt{2}}\right) \simeq 2.117\, a$

Example, $R = 10$, $a = 1$ fm

$R' = 10$, $a' = 2.117$



$g(r_m) = \frac{1}{\alpha}$ for $r_m = R_0 + a_g\sqrt{\log \alpha}$

α	r_m
[illegible]	[illegible]
[illegible]	[illegible]
[illegible]	[illegible]

$\ell(r) = \frac{1}{r}\frac{df}{dr} = \frac{1}{r a_0}\frac{X}{(1+X)^2}$ $X = \exp\frac{r-R_0}{a_0}$

$R_0 = r_0 A^{1/3}$

$\ell(R_0) = \frac{1}{4 R_0 a_0}$

* Compilation: F.G. PEREY, At. Data Nucl. Data Tab. 17(1976) 1

* Systematics: D.G., W.H., ...

"Reasonable" values of the parameters

Nucleons

Only as a guide !

Geometry (fm)   r   1.2 – 1.3

a   .45 – .7   greater if gaussian

Strength (MeV)

Real   (45 – 55) – (.2 – .3)*E

Im. surf.   (2 – 7) + (.3 –.5)*E, constant or slightly decreasing above 8–10 MeV

Im. vol. small below 10 MeV, constant or slightly increasing above

Spin–orbit   (4 – 10)

Ambiguities: $V\ r^2$
$W\ a$

Input

– Physical system: (m,z) + (M,Z), E ⟶ μ, k, η
– Optical model potential ⟶ form factors (geometry)
⟶ depths

$\Downarrow$

$\boxed{\text{Solve the radial Schroedinger equation}}$

Processing

1. Define the internal and external regions ⟶ matching radius
2. Ext. region ⟶ Coulomb functions
3. Int. region ⟶ step–by–step integration

] Numerical problems

4. Matching ⟶ partial scattering amplitudes

$\boxed{\eta_{\ell j}}$

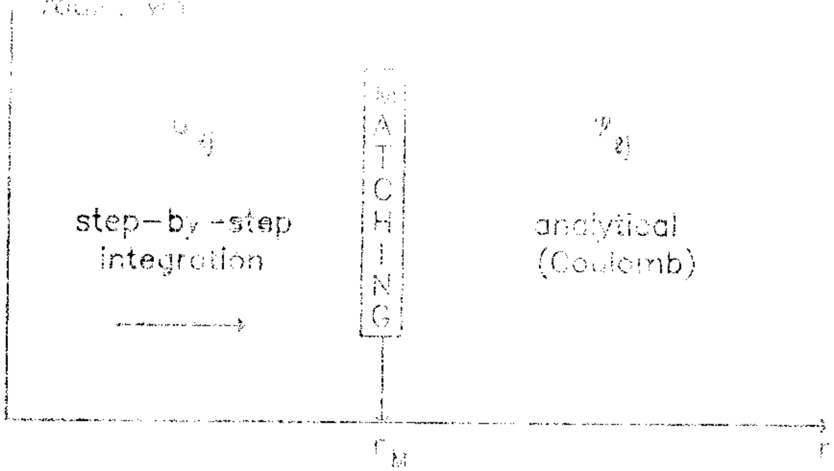
$\Downarrow$

Output

Transmission coefficients $T_{\ell j}$, T_ℓ (⟶ CN codes)

* Strength funct.: S_0, S_1
* Angular distributions $f(\theta,E)$, $a_\ell(E)$
* Cross sections
  – Total
  – Compound (⟶ CN codes)
  – Shape elastic (R')
* Polarisation $P(\theta,E)$

* Comparison with experimental data is possible.



$$\eta_\ell = S_\ell = \exp(2i\delta_\ell)$$

scattering amplitudes — phase shift

For the usual potential $U(r) = V f(r) = \frac{\varepsilon}{\alpha}$

$$\frac{1}{1+\exp\left(\frac{r-R}{a}\right)} = \frac{\varepsilon}{\alpha V}$$

$$\frac{r-R}{a} = \log\left(\frac{\alpha V}{\varepsilon}-1\right) \simeq \log\frac{\alpha V}{\varepsilon}$$

$$r_M = R + a\log\alpha + a\log\frac{V}{\varepsilon}$$

External region

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2}\,\frac{zZe^2}{r} - \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r)$$

remainder of the potential = Coulomb Term

$$\eta = z Z e^2/\hbar k$$

Change of variable $\rho = kr$

$$\left[\frac{d^2}{d\rho^2} + 1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{r}\right] u_\ell(\rho) = 0 \qquad \text{Coulomb eqn}$$

2 independant solutions: $F_\ell(\rho)$ regular

$G_\ell(\rho)$ irregular

If $\eta = 0$ (neutrons) and $u = \sqrt{\rho}\, w$

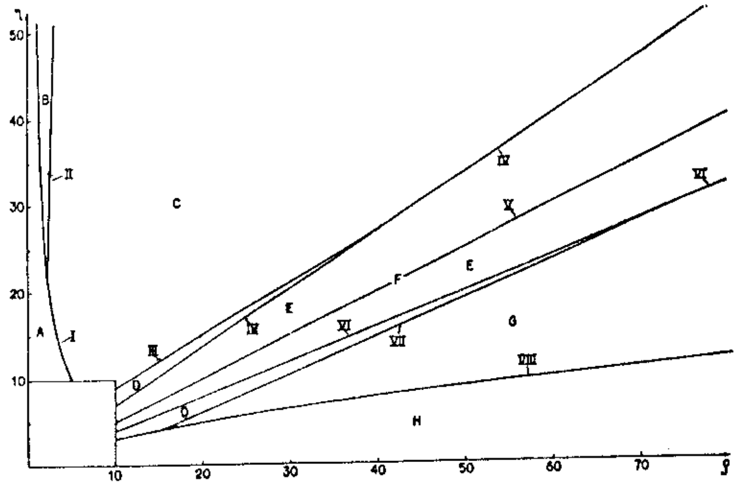
→ Bessel functions $J_{\pm(\ell+1/2)}$

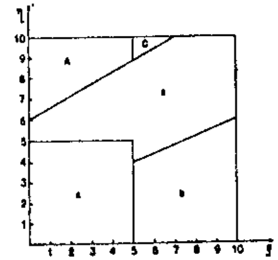
Previously, ≠ regions in the (η, ρ) plane to calculate F_ℓ and G_ℓ

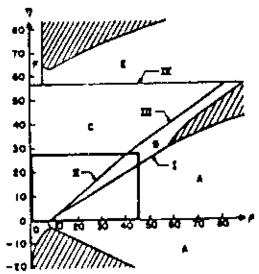
RCWFN: new technique by continued fraction calculations

→ only 2 regions for the whole plane

see A.R. BARNETT, Comp. Phys. Comm. 27 (1982) 147-166 and references therein.







- No explicit first derivative term → particularly suited for the method

$$u''(r) = f(r)\,u(r) \qquad (a)$$

- Uniform partition of $(0, r_M)$ $\qquad \Delta r = h = \frac{r_M}{N}$
- Taylor expansion

$$u(r+h) = u(r) + h\,u'(r) + \frac{h^2}{2!}\,u''(r) + \dots$$
$$u(r-h) = u(r) - h\,u'(r) + \frac{h^2}{2!}\,u''(r) + \dots$$

$$\rightarrow \quad u(r+h) - 2\,u(r) + u(r-h) = \frac{2h^2}{2!}\,u''(r) + \frac{2h^4}{4!}\,u^{(4)}(r)$$

- differentiate twice
- eliminate $u^{(4)}$
- use (a)
- putting $\quad y = u - \frac{h^2}{12}\,f u$

$$y(r+h) = 2\,y(r) - y(r-h) + h^2 f(r)\,y(r)$$

Numerov method $\rightarrow O(h^6)$

- fourth-order
- two-step
- explicit

- Initial conditions (in SCAT2) $\quad y(h) = \dots$
  $\quad y(2h) = \dots$

- Numerical errors: see Melkanoff et al.,
  Meth. in Comp. Phys. 6 (1966) 1.

Potential	Depth (MeV)	Radius (fm)	Diffus. (fm)
Real	50	1.25	.7
Imaginary surface	12	1.25	.7
Spin–orbit	7	1.25	.7