The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

1944-14

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

19 - 30 May 2008

exercises.

P. Descouvemont
Universite' Libre de Bruxelles
Brussels
Belgium

EXCEL PROGRAM rmatrix.xls

1. Introduction

The program solves the radial Schrödinger equation (positive or negative energies)

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)\psi_l(r)+V(r)\psi_l(r)=E\psi_l(r)$$

with the R matrix method. The coulomb $V_C(r)$ and nuclear $V_N(r)$ potentials are defined as (units are fm and MeV):

$V_C(r)=Z_1Z_2e^2/r$

$V_N(r)=V_0\exp(-(r/r_0)^2)$

For ^{12}C+p

ℓ=0,2: V_0=-73,8, r_0=2.7 (reproduce the ^{12}C+p resonance ($1/2^+$) energy 0.42 MeV)

ℓ=1: V_0=-55.3 (reproduce the ^{13}N ground state ($1/2^-$) energy -1.94 MeV)

For $\alpha+\alpha$

ℓ=0,2,4: V_0=-126, r_0=2.13 (reproduce the experimental phase shifts, from Buck et al. Nucl. Phys. A275 (1997) 246)

The wave function $\psi_l(r)$ is expanded over a set of *ng* basis functions as

$$\psi_l(r)=\sum_{i=1}^{ng}c_i^l u_i(r)$$

where c_i are linear coefficients. Here we use Gaussian functions

$$u_i(r)=r^l*\exp(-(r/a_i)^2),$$

with parameters $a_i=x_0*a_0^{(i-1)}$. Typical values are: x_0=0.6 fm, a_0=1.35.

The matrix elements of the Hamiltonian are computed analytically. Parameters (x_0,a_0) can be changed by the user (cells F7 and F8). The phase shifts are compared with the exact solutions.

Data to be entered (information is given in sheet "Help"):

- Masses (B1,D1), charges (B2,D2)
- V0 (B5), r0 (D5), ℓ (F5)
- Ng (B6)
- Channel radius rmax (B7)
- Number of energies (B8), initial energy E0 (B9), energy step EP (B10)

Outputs of the program

- *Phase shifts*
  column A: energy
  column B: exact phase shift
  column C: R-matrix phase shift
  column D: R matrix
  column E: exact derivative of the wave function at r=rmax

column F: left derivative of the R-matrix wave function at r=rmax
column G: right derivative of the R-matrix wave function at r=rmax
column H: 1/S(E), where S(E)=shift function
column I: hard-sphere phase shift
column J: penetration factor P(E)

- *Wave functions*
  Computed at the energy given in cell M11, and displayed in columns:
  column L: exact wave function
  column M: internal R-matrix wave function
  column N: external R-matrix wave function

- *Basis wave functions*
  Displayed in sheet "Wave func."

- *Potential*
  Displayed in sheet "Potential"

2. R-matrix formula

2.a General definitions

$$R(E) = \frac{\hbar^2 a}{2\mu} \sum_{ij} w_i^\ell(a) (D^\ell(E))^{-1}_{ij} w_i^\ell(a)$$

$$D^\ell_{ij}(E) = < u_i^\ell \; H + \mathcal{L}(0) \quad E | u_j^\ell >_{int} = \int_0^a u_i^\ell(r) \left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right) + \mathcal{L}(0) + V(r) \right] u_j^\ell(r) dr$$

$$U^\ell = \begin{matrix} I_\ell(ka) & 1 \\ O_\ell(ka) & 1 - LR^\ell \end{matrix}, \text{ with } L(E) = S(E) + iP(E)$$
$$= \exp(2i\delta^\ell) = \exp(2i(\delta^\ell_{HS} + \delta^\ell_R))$$

$$\exp(2i\delta^\ell_{HS}) = \frac{I_\ell(ka)}{O_\ell(ka)} \rightarrow \delta^\ell_{HS} = -\arctan \frac{F_\ell(ka)}{G_\ell(ka)}$$
$$\exp(2i\delta^\ell_R) = \frac{1 - L^* R^\ell}{1 - LR^\ell} \rightarrow \delta^\ell_R = \arctan \frac{PR}{1 - SR}$$

2.b Resonance energy E_r
In the R-matrix, E_r is a solution of $1-S(E_r)R(E_r)=0$
In the literature, the resonance energy E_r is also defined in different ways:

1) $\delta_R(Er)=90^o$ (corresponds to the definition above)
2) $\delta(Er)=90^o$
3) $d\sin\delta/dE)_{E=Er}=0$

For narrow resonances, the 4 definitions provide similar results.

2.c Resonance width Γ
In the R-matrix it is defined as

$$\tan \delta_R(E) \approx \frac{\Gamma}{2(E_r - E)}$$

3. Questions

3.1. For ^{12}C+p, ℓ=0 (narrow resonance):

1) Take x_0=0.6 fm and a_0=1.4, and choose a realistic R-matrix radius (rmax).
2) Compute the phase shifts up to 2 MeV for different numbers of basis functions (ng). Check out the left and right derivatives.
3) Increase and decrease rmax. Adapt ng accordingly.
4) Choose an energy, and compute (and plot) the wave function in good and poor conditions.
5) Verify the Thomas approximation (shift function *S(E)* linear near the resonance energy)
6) Determine approximately (by graphic) the resonance energy E_r by using the R-matrix definition above.
7) Determine approximately the resonance width.
8) Choose a good set (rmax, ng) and compute the phase shifts with the pole expansion. Verify that the phase shifts are identical.
9) With the pole energies E_λ and reduced widths γ_λ^2, determine (plot) both terms of

$$R(E) = \frac{\gamma_0^2}{E_0 - E} + R_0(E)$$

and verify that R_0(E) is almost constant.
Perform the same analysis for another *R*-matrix radius, and verify that both terms are sensitive to rmax (although the phase shift is not).

10) Compute the phase shifts with the first tem only (use *P(E)* and *S(E)* given in columns H and J). Evaluate the importance of the background term.

3.2. For α+α, ℓ=2 (broad resonance)
Repeat items1-2,9-10 of 3.1 up to 10 MeV. Show that the background term R_0(E) is more important than in 3.1 (narrow resonance).