Hands-on session on the R-matrix method:

Excel program talent_rmatrix_calc.xlsm

1. R-matrix formulae
2. Calculable R-matrix : general definitions
3. Writeup of the program rmatrix_calc.xlsm
4. Questions about the calculable R-matrix

1. R-matrix formulae

Note: all quantities depend on the angular momentum ℓ (not written)

Collision (or scattering) matrix : $U(E) = \frac{I(ka)}{O(ka)} \frac{1-L^{*}R(E)}{1-LR(E)} = \exp(2i\delta) = \exp(2i\delta_{HS}) \exp(2i\delta_{R})$

Hard-sphere phase shift: $\delta_{HS} = -\text{atan}\frac{F(ka)}{G(ka)}$

R-matrix phase shift: $\delta_{R} = \text{atan}\frac{P(E)R(E)}{1-S(E)R(E)}$

Incoming, outgoing Coulomb functions $I(x) = F(x) — G(x), O(x) = F(x) + iG(x)$, where $F(x)$ and $G(x)$ are the Coulomb functions

Penetration factor, shift factor defined from $L(E) = ka\frac{O'(ka)}{O(ka)} = S(E) + iP(E)$

Resonance energy E_r

In the R-matrix theory, the resonance energy 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) δ_R(Er)=90° (corresponds to the definition above)
2) δ(Er)=90°
3) $d\sin\delta/dE)_{E=Er}=0$

For narrow resonances, these definitions provide similar results.

2. Calculable R-matrix : general definitions

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

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right)u_\ell + (V_C(r)+V_N(r))u_\ell = Eu_\ell$$

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

$$V_C(r) = \frac{Z_1 Z_2 e^2}{r}$$

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

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

$$u_\ell(r) = \sum_{i=1}^{ng} c_{\ell,i}\phi_i(r),$$

where $c_{\ell,i}$ are linear coefficients. Here we use Gaussian functions

$$\phi_i(r) = r^\ell \exp(-(r/a_i)^2),$$

with parameters $a_i = x_0 \times a_0^{i-1}$. Typical values are: x_0=0.6 fm, a_0=1.4. 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.

The R-matrix is defined by

$$R(E) = \frac{\hbar^2 a}{2\mu}\sum_{ij}\phi_i(a)\,(C^{-1})_{ij}\phi_j(a)$$

$$C_{ij}(E) = <\phi_j|H - E + \mathcal{L}(0)|\phi_i>_{int}$$

$$= \int_0^a \phi_j(r)[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}\right) + V(r) + \mathcal{L}(0) - E]\phi_i(r)dr,$$

where $V(r)$ is the total potential (nuclear + Coulomb) and $\mathcal{L}(0)$ is the Bloch operator.

3. Writeup of the program rmatrix_calc.xlsm

Inputs

- Masses (B1,D1), charges (B2,D2)
- Parameters of the potential V_0 (B5), r_0 (D5), ℓ (F5)
- Number of basis functions ng (B6)
- Channel radius rmax (B7)
- Number of energies ne (B8), initial energy E0 (B9), energy step EP (B10)

Outputs

- *Phase shifts*
  column A: energy
  column B: “exact” phase shift (computed with the Numerov algorithm)
  column C: R-matrix phase shift
  column D: R matrix
  column E: exact derivative of the wave function $u_\ell(r)$ at r=rmax
  column F: left derivative of the R-matrix wave function $u_\ell(r)$ at r=rmax
  column G: right derivative of the R-matrix wave function $u_\ell(r)$ at r=rmax
  column H: $1/S_\ell(E)$, where $S_\ell(E)$=shift function
  column I: hard-sphere phase shift
  column J: penetration factor $P_\ell(E)$

- *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”

4. Questions about the calculable R-matrix

We consider the ^{12}C+p system (see Fig.1)

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

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

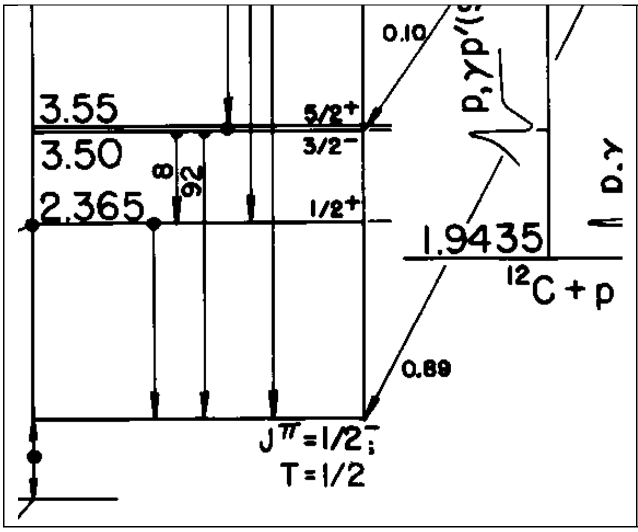

Fig.1 Experimental ^{13}N spectrum

a) Take x_0=0.6 fm and a_0=1.4, and choose a realistic R-matrix radius rmax (tabulate the potential).
b) Compute the phase shifts up to 2 MeV for different numbers of basis functions (ng). Check out the left and right derivatives.
c) Increase and decrease rmax. Adapt ng accordingly.
d) Choose an energy, and compute (and plot) the wave function in appropriate (ng large enough) and poor (ng too small) conditions.
e) Verify the Thomas approximation (shift function *S(E)* linear near the resonance energy)
f) Determine approximately (by graphic) the resonance energy E_r by using the R-matrix definition above (plot $R(E)$ and $1/S(E)$)
g) Choose an appropriate set (rmax, ng) and compute the phase shifts with the pole expansion. Verify that the phase shifts are identical.
h) 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 the background term $R_0(E)$ is approximately 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).
i) 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.