Computer Physics Communications 33 (1984) 421–424
North-Holland, Amsterdam

RESON – A PROGRAM FOR THE DETECTION AND FITTING OF BREIT-WIGNER RESONANCES

Jonathan TENNYSON and Cliff J. NOBLE

SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire WA4 4AD, UK

Received 12 March 1984; in revised form 24 May 1984

PROGRAM SUMMARY

Title of program: RESON

Catalogue number: ACCW

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application from in this issue)

Computer: NAS 7000; *Installation:* Daresbury Laboratory

Operating system: MVT

Programming language used: Fortran IV and Fortran 77

High speed storage required: 200 K

No. of bits in a byte: 8

Peripherals used: card reader, lineprinter, 2 disk files

No. of lines in program and test deck: 416 in RESON plus 4189 in NAG routines

Keywords: resonances, Breit–Wigner form, least squares-fitting

Nature of physical problem
RESON detects resonances in a list of eigenphase sums and fits them to a Breit–Wigner form.

Method of solution
The resonances are detected by sign changes in the second derivative of the energy with respect to the eigenphases. A least squares fit is then performed in the region of the resonance.

Restrictions on the complexity of the problem
RESON will only fit up to two overlapping resonances.

Typical running time
0.2 s per resonance on NAS 7000.

Unusual features of program
RESON uses NAG library minimisation routine E04FDF. It can also generate requests for fitting points to give a fully automated resonance detection and fitting package.

LONG WRITE-UP

1. Introduction

Resonances, or long-lived quasi-bound states lying in the continuum, are commonly found in many problems of physical interest such as nuclear interactions, heavy particle (atom–atom or molecule–molecule) scattering and electron–atom or molecule collision processes. These resonances manifest themselves in theoretical calculations as a rapid increase by π rad in the total eigenphase sum superimposed on a background eigenphase sum which varies slowly as a function of the scattering energy. They can be characterised by a position, $E^{\rm res}$, and width, $\Gamma^{\rm res}$. Within the Breit–Wigner form [1], the eigenphase (η) as a function of the scattering energy (E), is written for multiple resonances as:

$$\eta(E) = \sum_{i=1}^{M} \tan^{-1}\left[\frac{\Gamma_i^{\rm res}}{(E - E_i^{\rm res})}\right] + \sum_{i=0}^{N} a_i (E)^i. \quad (1)$$

The second summation in (1) is a power series to represent the underlying trend in the eigenphase across the region of the resonance. This background is usually represented by a linear ($N = 1$) or a quadratic ($N = 2$) energy dependence.

For many scattering problems, especially those involving charged particles very many resonances can occur. Fitting these by hand can be tedious and time consuming. We have thus implemented a procedure for automatically detecting and fitting resonances to a Breit–Wigner form.

2. Method

RESON reads a file of energy points and corresponding eigenphases. The second derivative, $d^2E/d\eta^2$, is constructed numerically and inspected for changes from positive to negative sign. This point is then marked as the location of a possible resonance and a fit is attempted. RESON can handle eigenphase sums which are smoothed (i.e. increase by π) across a resonance or discontinuous. RESON can fit either individual eigenphases or the eigenphase sum. However, narrow resonances may be missed if the energy grid is too coarse.

The resonance(s) detected are fitted by defining a fitting region of twice $\Gamma^{\rm res}$ about $E^{\rm res}$. RESON generates its own guesses for $\Gamma^{\rm res}$ and $E^{\rm res}$ based on the input eigenphases. Fitting points are obtained (a) from the input points in this region if more points are provided than parameters or (b) by generating a request to an external program for eigenphases at a grid of energies. The resonance parameters are calculated by a least squares fit. Resonances are fitted individually unless two grids overlap in which case a two resonance fit is attempted.

3. Program organisation and data input

3.1. Organisation

RESON requires NAMELIST input from the card reader and the eigenphase data from unit NFTS. This is then stored on scratchfile NFTI.

Subroutine EIGPHA(E, ETA, I), which is only called when GETETA .EQ. TRUE, is a user supplied routine which returns the eigenphase, ETA, for the Ith energy point E.

Subroutine E04FDF is a NAG library routine for multidimensional least-squares minimisation and the user is referred to the NAG reference manual [2]. However, the following comments on the error flag IFAIL are pertinent. E04FDF returns the following values for IFAIL [2]

IFAIL = 0 successful return;

IFAIL = 1 parameter outside range (will only occur in RESON if the fixed dimension arrays need increasing);

IFAIL = 2 Fitting has not converged. RESON automatically restarts the fit once;

IFAIL = 3 The final point does not satisfy the conditions for acceptance as a minimum, but no lower point could be found. Experience has shown that the parameters in this case are satisfactory;

IFAIL = 4 Unable to complete a singular value decomposition in a reasonable number of sub-iterations;

IFAIL = 5–8 Some doubt whether a true minimum has been found: IFAIL = 5 is

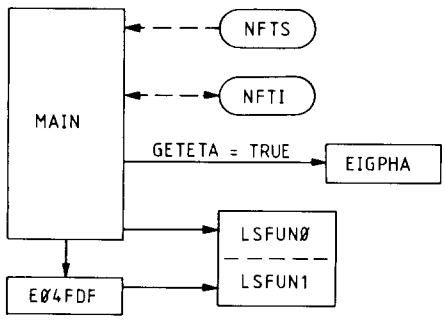

Fig. 1. Program structure.

probably a good estimate, IFAIL = 8 is unlikely to be a good estimate. Experience has shown answers with IFAIL $\leqslant$ 7 to be reliable.

Entry LSFUN1 is used by E04FDF for function evaluation, it is initiated by a calling subroutine LSFUN0, see fig. 1.

3.2. Card input

A single namelist /RESON/ is required. All data are defaulted (values given in square brackets). Note that whilst it is assumed that the eigenphases are in radians, the energy units are arbitrary.

NFTA [6] unit number of the line printer;

NFTS [9] unit number of the energy and eigenphase input data. This is read in one (E, ETA) pair per line with FORMAT (2D24.0);

NFTI [10] unit number of scratch file;

NRES [5] maximum number of resonances for which a fit is to be attempted;

NBACK [2] number of terms used to fit the background. NBACK = N + 1 (see eq. (1));

GETETA [.FALSE.]
Logical variable:
.TRUE. subroutine EIGPHA is to be called to generate the fitting points,
.FALSE. if the fitting points are to be taken from the input data;

IFLAG [0] Print flag:
= 0 for minimal printing;
= 1 for fuller printout,
= 2 for debug printing (use with caution).

4. Test cases

Test data for both GETETA = .TRUE. and .FALSE. are provided from results on e–H_2^+ scattering [3]. The resonance to be fitted corresponds to the lowest resonance of $^1\Sigma_g$ symmetry.

Acknowledgement

We are grateful to NAG for permission to include their routines.

References

[1] G. Breit and E.P. Wigner, Phys. Rev. 49 (1936) 519, 642.
A. Hazi, Phys. Rev. A19 (1979) 920.
[2] NAG Fortran Library Manual, Mark 10, vol. 3 (1983).
P.E. Gill and W. Murray, SIAM J. Num. Analysis 15 (1978) 977.
[3] J. Tennyson, C.J. Noble and S. Salvini, J. Phys. B17 (1984) 905.

TEST RUN OUTPUT

```
   30 ENERGY POINTS READ IN
ENERGY=   0.35000 ETA=    0.511524 0743D+00
ENERGY=   0.36000 ETA=    0.606796 2643D+00 SECOND DERIV=    0.841978862 0D-01
ENERGY=   0.37000 ETA=    0.721349 6337D+00 SECOND DERIV=    0.561842502 2D-01
ENERGY=   0.38000 ETA=    0.857994 9892D+00 SECOND DERIV=    0.354874921 2D-01
ENERGY=   0.39000 ETA=    0.101756 0002D+01 SECOND DERIV=    0.203093570 4D-01
ENERGY=   0.40000 ETA=    0.119680 5672D+01 SECOND DERIV=    0.877003438 2D-02
ENERGY=   0.41000 ETA=    0.138710 6355D+01 SECOND DERIV=   -0.104216310 7D-02
ENERGY=   0.42000 ETA=    0.157598 6642D+01 SECOND DERIV=   -0.110317955 6D-01
ENERGY=   0.43000 ETA=    0.175153 6404D+01 SECOND DERIV=   -0.230715863 8D-01
ENERGY=   0.44000 ETA=    0.190636 7940D+01 SECOND DERIV=   -0.389599912 4D-01
ENERGY=   0.45000 ETA=    0.203836 1896D+01 SECOND DERIV=   -0.603355881 3D-01
ENERGY=   0.46000 ETA=    0.214898 2199D+01 SECOND DERIV=   -0.885608331 3D-01
ENERGY=   0.47000 ETA=    0.224126 0223D+01 SECOND DERIV=   -0.124598573 2D+00
ENERGY=   0.48000 ETA=    0.231848 7303D+01 SECOND DERIV=   -0.168890 6065D+00
ENERGY=   0.49000 ETA=    0.238362 0488D+01 SECOND DERIV=   -0.221238566 2D+00
ENERGY=   0.50000 ETA=    0.243910 8926D+01 SECOND DERIV=   -0.280688491 3D+00
ENERGY=   0.51000 ETA=    0.248690 7943D+01 SECOND DERIV=   -0.345424415 2D+00
ENERGY=   0.52000 ETA=    0.252855 6116D+01 SECOND DERIV=   -0.412679626 2D+00
ENERGY=   0.53000 ETA=    0.256526 1259D+01 SECOND DERIV=   -0.478675781 8D+00
ENERGY=   0.54000 ETA=    0.259797 6163D+01 SECOND DERIV=   -0.536347658 2D+00
ENERGY=   0.55000 ETA=    0.262747 1438D+01 SECOND DERIV=   -0.592132988 3D+00
ENERGY=   0.56000 ETA=    0.265432 4080D+01 SECOND DERIV=   -0.613248203 9D+00
ENERGY=   0.57000 ETA=    0.267907 3629D+01 SECOND DERIV=   -0.620440 9387D+00
ENERGY=   0.58000 ETA=    0.270213 0570D+01 SECOND DERIV=   -0.591383490 3D+00
ENERGY=   0.59000 ETA=    0.272386 0485D+01 SECOND DERIV=   -0.522366298 2D+00
ENERGY=   0.60000 ETA=    0.274459 1239D+01 SECOND DERIV=   -0.407783441 6D+00
ENERGY=   0.61000 ETA=    0.276463 1289D+01 SECOND DERIV=   -0.244674552 3D+00
ENERGY=   0.62000 ETA=    0.278428 8710D+01 SECOND DERIV=   -0.344288804 3D-01
ENERGY=   0.63000 ETA=    0.280389 4035D+01 SECOND DERIV=    0.215024992 3D+00
ENERGY=   0.64000 ETA=    0.282383 1719D+01
1
 AUTOMATIC RESONANCE FITTING:
    1 RESONANCES DETECTED
    1 RESONANCES TO BE FITTED

RESONANCE  1 IN THE RANGE ELOW=   0.32715 TO EHIGH=   0.49285

GRID POINT   1 E=   0.35000 ETA=    0.511524 0743D+00
GRID POINT   2 E=   0.36000 ETA=    0.606796 2643D+00
GRID POINT   3 E=   0.37000 ETA=    0.721349 6337D+00
GRID POINT   4 E=   0.38000 ETA=    0.857994 9892D+00
GRID POINT   5 E=   0.39000 ETA=    0.101756 0002D+01
GRID POINT   6 E=   0.40000 ETA=    0.119680 5672D+01
GRID POINT   7 E=   0.41000 ETA=    0.138710 6355D+01
GRID POINT   8 E=   0.42000 ETA=    0.157598 6642D+01
GRID POINT   9 E=   0.43000 ETA=    0.175153 6404D+01
GRID POINT  10 E=   0.44000 ETA=    0.190636 7940D+01
GRID POINT  11 E=   0.45000 ETA=    0.203836 1896D+01
GRID POINT  12 E=   0.46000 ETA=    0.214898 2199D+01
GRID POINT  13 E=   0.47000 ETA=    0.224126 0223D+01
GRID POINT  14 E=   0.48000 ETA=    0.231848 7303D+01
GRID POINT  15 E=   0.49000 ETA=    0.238362 0488D+01

INITIAL VALUES FOR FITTING PROCEDURE

RESONANCE  1 FIT:
ERES =       0.41 0000000D+00  GAMMA =       0.828520 65D-01
BACKGROUND:       0.0                  0.0

FIT COMPLETE, RESIDUES:
    0.0003404   -0.0000187   -0.0002181   -0.0002496   -0.0001355    0.0000530    0.0002057    0.0002328    0.0001253   -0.0000503
   -0.0002064   -0.0002738   -0.0002098    0.0000089    0.0003961

RESONANCE  1 FIT:
ERES =       0.409 00363D+00  GAMMA =       0.105910 95D+00
BACKGROUND:      -0.32254552D+00       0.29228479D+00
```