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MEATPI AND SORCE. TWO PROGRAMS TO CALCULATE SCATTERING POTENTIALS FROM PHASE SHIFTS

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Abstract

A description is given of the computer programs MEATPI and SORCE which calculate an effective two body potential. Reaction matrix parameters are calculated in MEATPI from the input phase shifts and SORCE then uses these parameters to generate the potential.

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BOUNDARY CONDITIONS; LEAST SQUARE FIT; M CODES; PHASE SHIFT; POTENTIAL SCATTERING; R MATRIX; S CODES; S MATRIX; SQUARE-WELL POTENTIAL; TWO-BODY PROBLEM; WAVE FUNCTIONS

CONTENTS

1. INTRODUCTION

In the Inverse Reaction problem we try to discover the extent to which the scattering potential is determined from an assignment of the phase shifts. For a discussion of this problem see Newton (1966, Chap. 20) or the review article by Faddeyev (1963). The programs MEATPI and SORCE were written to apply a method suggested by Cook (1970), who showed that the potential could be written as a ratio of two series of simple functions; the coefficients of expansion being given by reaction matrix theory. In MEATPI the scattering phase shifts are used to generate a set of resonance parameters. These are then used in SORCE to calculate the potential. Listings of these programs are available from the author.

2. THEORY

In these calculations we are seeking solutions of the wave equation:

$$\left[\frac{d^2}{dr^2} + q^2 - V(q,r) - \frac{\ell(\ell+1)}{r^2}\right] \Psi(q,r) = 0 \quad , \qquad \ldots(1)$$

which may be expanded in terms of a complete orthonormal set of eigenfunctions $U_\lambda(r)$ by the series:

$$\Psi(q,r) = \sum_\lambda A_\lambda(q) U_\lambda(r) \quad . \qquad \ldots(2)$$

$U_\lambda(r)$ satisfies the eigenvalue equation

$$\left[\frac{d^2}{dr^2} + q_\lambda^2 - V(q,r) - \frac{\ell(\ell+1)}{r^2}\right] U_\lambda(r) = 0 \quad , \qquad \ldots(3)$$

and the boundary conditions

$$\left.\frac{dU_\lambda(r)}{dr}\right|_{r=a} = \frac{B_\ell}{a} U_\lambda(a) \qquad \ldots(4)$$

where short range forces have been chosen so that

$$V(q,r) = 0 \qquad r>a \quad . \qquad \ldots(5)$$

The essential point of this method is that we may write the reaction matrix R in terms of these eigenfunctions:

$$R = \frac{1}{a}\sum_\lambda \frac{U_\lambda^2(a)}{q_\lambda^2-q^2} = \sum_\lambda \frac{\gamma_\lambda^2}{q_\lambda^2-q^2} \qquad \ldots(6)$$

where $\gamma_\lambda^2 = \dfrac{U_\lambda^2(a)}{a}$.

The widths γ_λ^2 and the poles q_λ^2 may be determined from the phase shifts. The background to any of the reaction matrix theory used here is given by Preston (1962, Chap. 16) or by Lane and Thomas (1958).

In this section a brief outline of the reaction matrix method of Cook (1970) is given. Rewrite the wave equation (1) as a source equation

$$\left[\frac{d^2}{dr^2} + q^2 - \frac{\ell(\ell+1)}{r^2}\right] \Psi(q,r) = \rho(q,r) \quad . \qquad \ldots(7)$$

Assume that the physical solution $\Psi(q,r)$ and the source $\rho(q,r)$ may be expanded

$$\Psi(q,r) = \sum_\lambda A_\lambda(q) U_\lambda(r)$$

$$\rho(q,r) = \sum_\lambda A_\lambda(q) \rho_\lambda(r) \qquad \ldots(8)$$

where $U_\lambda(r)$ forms a complete orthonormal set which is the solution of the eigenvalue equation

$$(\nabla^2 + q_\lambda^2) U_\lambda(r) = \rho_\lambda(r) \quad , \qquad \ldots(9)$$

with the boundary conditions

$$\left.\frac{dU_\lambda(r)}{dr}\right|_{r=a} = \frac{B_\ell}{a} U_\lambda(a) \quad . \qquad \ldots(10)$$

The radius a is chosen such that the short range interaction vanishes, that is

$$\rho_\lambda(r) = 0 \qquad r>a$$

$$\rho(q,r) = 0 \qquad r>a \quad . \qquad \ldots(11)$$

We could also solve (7) for $\rho = 0$ and with the boundary conditions (10) to obtain a complete orthonormal set of free particle eigenfunctions $W_\mu(r)$ where

$$(\nabla^2 + k_\mu^2) W_\mu(r) = 0 \quad , \qquad \ldots(12)$$

and k_μ^2 are the discrete eigenvalues obtained from $W_\mu(r)$.

The first problem is to determine $U_\lambda(r)$ and $\rho_\lambda(r)$ in (8). Cook assumed that they may be expanded in terms of $W_\mu(r)$ by

$$U_\lambda(r) = \sum_\mu B_{\lambda\mu} W_\mu(r)$$

$$\rho_\lambda(r) = \sum_\mu C_{\lambda\mu} W_\mu(r) \qquad \ldots(13)$$

Substituting (13) in (9) and applying Green's theorem to (12) and (9) gives

$$(q_\lambda^2 - k_\mu^2) B_{\lambda\mu} = C_{\lambda\mu} \quad . \qquad \ldots(14)$$

Thus once the matrix $\underline{B}$ is determined we may obtain $\underline{C}$ and thus U_λ and ρ_λ. To calculate the wave function and the source term we now have to find A_λ.

Applying Green's theorem to (8) and (9) gives

$$A_\lambda(q) = \frac{1}{aR} \frac{U_\lambda(a)\Psi(q,a)}{q_\lambda^2 - q^2} \qquad \ldots(15)$$

where

$$\Psi(q,a) = j_\ell(q\,a) - K(q) n_\ell(q\,a) \qquad \ldots(16)$$

and

$$K(q) = -\frac{1}{q}\int_0^a j_\ell(q\,r)\rho(q,r)dr = \tan\delta \quad , \qquad \ldots(17)$$

where δ is the phase shift.

It is convenient to calculate $\underline{B}$ from the eigenvalues on the boundary as $U_\lambda^2(a)$ is determined from the parameters of the reaction matrix. As both $U_\lambda(r)$ and $W_\mu(r)$ form complete orthonormal sets, $\underline{B}$ is a unitary matrix and we have

$$\sum_\lambda U_\lambda^2(a) = \sum_\mu W_\mu^2(a) \quad . \qquad \ldots(18)$$

B is written as a bilinear form

$$B_{\lambda\mu} = \frac{1}{(U.U-U.W)}\left[U_\lambda(a)W_\mu(a)+U_\mu(a)W_\lambda(a)-U_\lambda(a)U_\mu(a)-W_\mu(a)W_\lambda(a)\right]+\delta_{\lambda\mu} \qquad \ldots(19)$$

An 'effective' energy dependent, local potential may be defined by

$$V(q,r) = \frac{\rho(q,r)}{\Psi(q,r)} = \frac{\sum\limits_{\lambda\mu} A_\lambda(q) C_{\lambda\mu} W_\mu(r)}{\sum\limits_{\lambda\mu} A_\lambda(q) B_{\lambda\mu} W_\mu(r)} \quad . \qquad \ldots(20)$$

This potential may be replaced by an energy independent non local potential (see Mott and Massey 1965, p. 183). For these programs this has not been done but it may prove useful for future calculations.

To apply these methods we must know the widths γ_λ^2 and the poles q_λ^2 of the reaction matrix. To calculate these parameters follow Preston (1962) and consider the definition of the scattering matrix S_ℓ for each partial wave.

$$S_\ell = e^{2i\delta_\ell} = \frac{nP^{\frac{1}{2}}(1-R_\ell L_\ell^*)P^{-\frac{1}{2}}n}{1-R_\ell L_\ell} \qquad \ldots(21)$$

where the logarithmic derivative quantity L_ℓ may be written

$$L_\ell = s_\ell + ip_\ell \qquad \ldots(22)$$

and

$$n = e^{-2i\omega}$$

$$\delta = \alpha - \omega \quad .$$

ω is the hard sphere phase shift, p_ℓ is the penetration factor and s_ℓ is the level shift as defined by Preston. As short range forces have been assumed p_ℓ, s_ℓ and ω may be evaluated from the free particle wave functions $j_\ell(q\ a)$ and $n_\ell(q\ a)$.

Subtracting the hard sphere phase and taking the real and imaginary parts of (21) gives

$$\tan\alpha = R_\ell p_\ell/(1-R_\ell s_\ell)$$

and hence

$$R_\ell = \tan\alpha/(p_\ell+s_\ell \tan\alpha) \quad . \qquad \ldots(23)$$

We may take account of the non-zero boundary conditions in (10) by introducing the boundary condition

$$B_\ell = -\ell \qquad \ldots(24)$$

which modifies the definition of R_ℓ given above to

$$R_\ell = \tan\alpha/(p_\ell + \left(s_\ell - B_\ell\right)\tan\alpha) \quad . \qquad \ldots(25)$$

For these calculations the reaction matrix was written as

$$R = R_o + \sum_{\lambda=1}^{N} \frac{\gamma_\lambda^2}{q_\lambda^2 - q^2} \quad . \qquad \ldots(26)$$

From the input phases δ, R_ℓ was calculated from (25). This was then least squares fitted to (26) to find the poles q_λ^2 and widths γ_λ^2.

3. SOME NUMERICAL CONSIDERATIONS

The main difficulty in applying reaction matrix techniques to the inverse reaction problem is that from a least squares fit to the phase shifts only a finite number of poles q_λ^2 and widths γ_λ^2 are found. As the complete spectrum is not known we have to resort to approximations to calculate the effect of the background R_o on the potential.

For the calculations in MEATPI and SORCE it was assumed that for energies outside the region of interest the potential is a square well of depth $-V_o$. For this potential we may write the wave function and reaction matrix exactly. The advantage of the square well is that the widths in the reaction matrix are the same as for the free particle widths and the pole positions are easily calculated from the free particle poles.

Using this approximation, the reaction matrix, source term and wave function are written as a sum over the known poles with contributions from the square well. We then write

$$\rho(q,r) = \frac{\Psi(q,a)}{aR} \left\{ \left[\sum_{\lambda=1}^{N+1} \frac{U_\lambda(a)\rho_\lambda(r)}{q_\lambda^2 - q^2} + V_o \frac{W_\lambda(a)W_\lambda(r)}{k_\lambda^2 - V_o - q^2} \right] - V_o \frac{aR_{s.w.}}{\Psi_{s.w.}} j_\ell(\phi\, r) \right\} \qquad \ldots(27)$$

$$\Psi(q,r) = \frac{\Psi(q,a)}{aR} \left\{ \left[\sum_{\lambda=1}^{N+1} \frac{U_\lambda(a)U_\lambda(r)}{q_\lambda^2 - q^2} - \frac{W_\lambda(a)W_\lambda(r)}{k_\lambda^2 - V_o - q^2} \right] + \frac{aR_{s.w.}}{\Psi_{s.w.}} j_\ell(\phi\, r) \right\} \qquad \ldots(28)$$

$$R = \sum_{\lambda=1}^{N+1} \frac{\gamma_\lambda^2}{q_\lambda^2 - q^2} + R_{s.w.} - \sum_{\lambda=1}^{N+1} \frac{\delta_\lambda^2}{k_\lambda^2 - V_o - q^2} \qquad \ldots(29)$$

where $\phi = \sqrt{q^2 + V_o}$

$$R_{s.w.} = \frac{j_\ell(\phi\, a)}{\phi a j_{\ell-1}(\phi\, a)}$$

$$\Psi_{s.w.} = j_\ell(\phi\ a)$$

$$\Psi(q,a) = j_\ell(q\ a) - \tan\delta\ n_\ell(q\ a)$$

$$\delta^2_\lambda = \frac{W^2_\lambda(a)}{a} = \text{square well width.}$$

These approximations are also used to calculate the reaction matrix from the phase shifts. The form (26) for the reaction matrix does not guarantee the unitarity of $\underline{B}$. To ensure this an extra pole is used. This accounts for the sum over N+1 terms in (27), (28) and (29). The fixing of the parameters for the extra pole is as follows:

Its width is calculated from (18), taking the sum to N+1 terms, giving

$$\gamma^{\ 2}_{N+1} = \sum_{\mu=1}^{N+1} \delta^2_\mu - \sum_{\mu=1}^{N} \gamma^2_\mu \ . \qquad \ldots(30)$$

The depth of the square well potential is taken to be

$$V_o = k^2_1 - q^2_1 \qquad \ldots(31)$$

The depth was calculated from the difference between the lowest energy free particle pole and the lowest energy interaction pole. This is a somewhat arbitrary assignment but it was used because the lowest pole is normally well known and thus (31) will produce a more accurate estimation of the depth of the background potential than performing this sum for all pairs and then averaging.

We now have only to find the position of the N+1th pole. This is done by a least squares fit. If we define

$$R_B = R_{s.w.} - \sum_{\mu=1}^{N+1} \frac{\delta^2_\mu}{k^2_\mu - V_o - q^2} \qquad \ldots(32)$$

then (29) may be least squares fitted over all the energy points to give

$$q^2_{N+1} = \frac{\sum_i q^2_i (R^1_i - f_i)^2 + \gamma^2_{N+1} \sum_i (R'_i - f_i)}{\sum_i (R'_i - f_i)} \qquad \ldots(33)$$

where $$f_i = \sum_{\lambda=1}^{N} \frac{\gamma_\lambda^2}{q_\lambda^2 - q^2}$$

$$R_i' = R_i - R_{B_i}$$

and R_i is calculated from (25) at each energy point q_i^2. These extra parameters, together with (29) for the definition of R guarantee the unitarity of $\underline{B}$.

The free particle eigenfunctions $W_\mu(r)$ are given by

$$W_\mu(r) = N\, j_\ell(k_\mu r) \qquad \ldots(34)$$

where N is a normalization constant to ensure the $W_\mu(r)$ are orthonormal. It may be determined by the equation (Erdelyi, 1953 p. 71)

$$\int_0^1 t\, J_u^2 \left(\lambda_m t\right) dt = \tfrac{1}{2}\, \bar{\lambda}_m^{2} \left\{ \lambda_m^2 \left[J_u^1 \left(\lambda_m\right)\right]^2 + \left(\lambda_m^2 - U^2\right) J_u^2 \left(\lambda_m\right) \right\} \qquad \ldots(35)$$

where $\lambda_m = k_m a$.

After some tedious manipulation this gives

$$N = \left(\frac{2}{a j_\ell^2 \;(k_\mu a)}\right)^{\frac{1}{2}} . \qquad \ldots(36)$$

k_μ is found from the recurrence relations for the Riccati-Bessel functions.

$$j_{\ell-1}(z) = \frac{dj_\ell(z)}{dz} + \ell j_\ell(z)/z \qquad \ldots(37)$$

With the boundary conditions (10) and (24) this immediately shows that k_μ is such that

$$j_{\ell-1}(k_\mu a) = 0 \qquad \ldots(38)$$

A simple Regula Falsi calculation gives the zeros of $j_{\ell-1}(z)$ and thence k_μ.

The functions $j_\ell(z)$ were calculated with the series expansion of Schelkunoff (1951, p. 397).

$$j_\ell(z) = \sin\left(z - \frac{\pi}{2}\right) A_\ell + \cos\left(z - \frac{\pi}{2}\right) B_\ell \qquad \ldots(39)$$

$$n_\ell(z) = \sin\left(z - \frac{\pi}{2}\right)B_\ell - \cos\left(z - \frac{\pi}{2}\right)A_\ell \qquad \ldots(39)$$

where
$$A_\ell(z) = \sum_{m=0}^{2m\leq\ell} \frac{(-1)^m\ (\ell+2m)!}{(2m)!\ (\ell-2m)!\ (2z)^{2m}}$$

$$B_\ell(z) = \sum_{m=0}^{2m\leq\ell-1} \frac{(-1)^m\ (\ell+2m+1)!}{(2m+1)!\ (\ell-2m-1)!\ (2z)^{2m+1}}$$

After these functions are given it is a simple matter to calculate ω from

$$\omega = -\tan^{-1}\frac{j_\ell(qa)}{n_\ell(qa)} \quad . \qquad \ldots(40)$$

The penetration factors and level shifts are given by the recurrence relations (Lane and Thomas 1958)

$$p_\ell = bp_{\ell-1}\Big/\left[\left(\ell-s_{\ell-1}\right)^2 + p^2_{\ell-1}\right]$$

$$s_\ell = b\left(\ell-s_{\ell-1}\right)\Big/\left[\left(\ell-s_{\ell-1}\right)^2 + p^2_{\ell-1}\right] - \ell \qquad \ldots(41)$$

where
$$b = (qa)^2 \quad p_0 = qa \quad s_0 = 0 \quad .$$

Once the source and potential have been found they may be checked by recalculating the phase shift. Two methods were considered; firstly the integration over the source as defined by (17) and secondly a standard phase shift analysis.

For the first method a simple trapezoidal integration sufficed. This produced accurate results with a relatively large step size. In the phase shift analysis the wave equation (1) was numerically integrated from the origin using a central difference method (Fox 1962, p. 39).

$$\left(1 - \frac{1}{12}h^2 f_{n+1}\right)y_{n+1} = \left(2 + \frac{5}{6}h^2 f_n\right)y_n - \left(1 - \frac{1}{12}h^2 f_{n-1}\right)y_{n-1} \qquad \ldots(42)$$

where h is the step length and
$$f_n = -\left\{q^2 - V(q,r_n) - \frac{\ell(\ell+1)}{r_n^2}\right\} \quad .$$

Two starting values were provided by the series expansion (8). The solution obtained from the integration was matched onto $j_\ell(qr)$ and $n_\ell(qr)$ outside the region of interaction and the phase shift obtained. This method proved to be somewhat more difficult because of discontinuities in the potential. To provide the same accuracy as the source integration required a much smaller step size. As this necessitated a longer computing time it was not used.

4. INPUT/OUTPUT SPECIFICATIONS

MEATPI

I) INPUT

Card 1	FORMAT (2D10.3)
AMAS1	mass of the target in MeV
AMAS2	mass of the incident particle in MeV
Card 2	FORMAT (2D10.3)
RMIN	minimum value of the radius
RMAX	maximum value of the radius (Both in Compton wavelengths)
Card 3	FORMAT (5X,2I2)
NMIN	minimum number of poles N in the reaction matrix
NMAX	maximum number of poles in the reaction matrix
Card 4	FORMAT (5A4,I3)
TITLE	used to give a description of the run
L	the value of the orbital angular momentum for the partial wave considered
Card 5 onwards	FORMAT (2D10.3)
ELAB	energy of the incident particle in the laboratory frame in MeV
A	value of the phase shift in degrees at that energy.

For each value of ELAB, q which is the centre of mass momentum of the incident particle is calculated using the relativistic transformations of Bethe and De Hoffmann (1955, p. 402).

Last Card BLANK

This delimits the input data. If more than one partial wave is required the cards from TITLE (Card 4) onward are then repeated.

II) OUTPUT

For each value of the radius a the reaction matrix parameters are calculated for N between NMIN and NMAX. The radius is then increased by 0.1 Compton wavelengths and the calculation repeated until RMAX is reached. The output has the form

```
TITLE ............... L = ....... RADIUS = .......
INPUT DATA
     ELAB      PHASE
     ....      .....
     ....      .....
```

Then follows

```
     ELAB       P        S        HS
     ....      ....     ....     ....
     ....      ....     ....     ....
```

where P is the penetration factor, S the level shift and HS the hard sphere phase shift.

For each value of N the output is as follows

```
NO. OF POLES = .......
     R MATRIX PARAMETERS
     Q**2           GAMMA **2
     ....           .........         There are N+1 poles returned from
     ....           .........         the calculation
        VO = .......
```

VO is in units of the incident particle rest mass.

```
     LEAST SQUARES FIT
     Q**2       R        RCAL       DIFF       CHI
     ....      ....      ....       ....       ....
     ....      ....      ....       ....       ....
     ....      ....      ....       ....       ....
        CHI**2 = ....
```

where R is the input reaction matrix calculated from (25) and RCAL is the least squares fitted matrix (29).

```
     RECALCULATED VALUES
     ELAB        PHASE        CALC
     ....        .....        ....
     ....        .....        ....
     ....        .....        ....
```

SORCE

I) INPUT

Card 1 FORMAT (7X,2D10.3)

AMAS1

AMAS2

(These are the same as for MEATPI)

Card 2	FORMAT (7X, 2D10.3)
DUNL	smallest value of r for which the potential is evaluated
DUNIN	step length in r

(Both in Compton wavelengths)

Card 3	FORMAT (5A4,I3)
TITLE	
L	

(These are the same as for MEATPI)

Card 4 onwards	FORMAT (2D10.3)
ELAB	
A	

(These also are the same as for MEATPI)

Card 5	Blank

(This delimits the energy data)

Card 6	FORMAT (2D10.3)
RAD	the interactive range a, in Compton wavelengths
VO	the depth of the square well potential
Card 7 onwards	FORMAT (7X, 2D10.3)
ER	position of the pole in the reaction matrix
GN	width of the pole

There are N+1 of these

Card 8	Blank

(This delimits the resonance parameter data)

If more than one partial wave is being considered the cards from TITLE (Card 3) have to be repeated.

II) OUTPUT

For each set of resonance parameters the potential is calculated and printed at DUNL and then at values of r increasing by DUNIN until RAD is reached. This process is repeated for all values of the incident energy. The output has the form

```
TITLE ...........     L = .........
FREE     PARTICLE     MOMENTUM     SQUARED
....       ....         ....         ....
```

```
     RESONANCE     ENERGY     AND     WIDTH
         ....                 ....
         ....                 ....
         ....                 ....
WELL DEPTH = .......
INTERACTION RANGE TAKEN AS ..... C.W.
EIGENVALUES FROM R MATRIX
.....   .....   .....   ....
EIGENVALUES AT BOUNDARY
....   ....   ....   ....
```

The eigenvalues at the boundary are calculated from the unitary matrix B̲.

```
     LAB.ENERGY (MeV) = ....  Q**2 = ....
        V(Q,R)     R     PSI     RHO
        .....     ....   ....    ....
        .....     ....   ....    ....
        .....     ....   ....    ....
        .....     ....   ....    ....
```

This last output block is repeated for all the incident energies ELAB.

V(Q,R) is given in units of the incident particle rest mass.

```
     FINAL OUTPUT
     LAB ENERGY       INPUT       CALC
         ....          ....       ....      ....
         ....          ....       ....      ....
         ....          ....       ....      ....
```

There are two columns of calculated output. The first is the phase calculated from the integration over the source; the second is the phase calculated from the reaction matrix parameters.

5. ACKNOWLEDGMENTS

I would like to thank Mr. J. Cook and Dr. B. Clancy for many useful discussions throughout this work. I would also like to thank Mr. G. Trimble for help with the computing.

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