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A GENERAL PROGRAM FOR CALCULATING CROSS-SECTIONS
IN WAVE MECHANICS

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A GENERAL PROGRAM FOR CALCULATING CROSS-SECTIONS IN WAVE MECHANICS

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ABSTRACT

The wave mechanical cross-section formulae for one incident channel and N exit channels are derived in matrix form. A method for calculating these cross sections is discussed and a listing of the Fortran program used on an IBM-704 is given. As an illustration, the program is used to calculate cross sections obtained in the weak coupling approximation in the scattering of positrons by atomic hydrogen.

I. INTRODUCTION

In the wave mechanical description of a scattering process, for example the elastic or inelastic scattering of electrons from hydrogen atoms,⁽¹⁾ or the elastic scattering of protons by tritons,⁽²⁾ the first step in the analysis, after writing down the Schrödinger equation for the problem, is to expand the total wave function, Ψ , in terms of the complete set of eigenfunctions, ϕ_n say, of the target Hamiltonian. The expansion coefficients, $F_n(\underline{r})$ say, are then interpreted as describing the motion of the incident projectile relative to the target particle in its various quantum states. The boundary conditions imposed on the coefficients are:

$F(0)$ finite

$$F_n(\underline{r}) \sim e^{i\mathbf{k}_n \cdot \underline{r}} \delta_{ni} + \frac{e^{i\mathbf{k}_n \cdot \underline{r}}}{r} g_{in}(\theta, \phi) \quad , \quad (I.1)$$

where the suffix "i" denotes the initial state, or states, of the target particle and $\cos \theta \equiv \mathbf{k}_n \cdot \mathbf{k}_i$. Using the wave mechanical expression for the flux of particles,⁽⁵⁾ the total cross sections are given by

$$Q_{in} = \frac{k_n}{k_i} \int_0^{2\pi} \int_0^\pi d\phi \sin \theta d\theta |g_{in}(\theta, \phi)|^2 \quad . \quad (I.2)$$

In this report, it is assumed that all the target particles are initially in one definite quantum state; hence, the suffix i will only have one

value, t say, i.e., we consider only one entrance channel. However, n can take on any number of values from 1 to N, depending upon the number of terms, N, taken in the expansion for Ψ . Until digital computing machines, with large storage and high speed, became generally available, the amount of numerical work required to solve the differential equations for the $F(\underline{r})$ was so large as to limit investigations to $N = 1$ and occasionally to $N = 2$.⁽¹⁾ Thus, it was sufficient to derive analytic expressions for the Q_{tn} of Eq. (I.2) up to $N = 2$. For $N \geq 3$, i.e., for three or more coupled equations in $F_n(\underline{r})$, the explicit forms of Q_{tn} are so complicated that another method must be used to derive these expressions.

In Sec. (II), a general expression for the cross section for single-entrance channel processes is derived. The analysis of this expression for Fortran programming is described in Sec. (III). The Fortran listing for $N = 3$ is given in Sec. (IV) and is used with results obtained from calculations in the weak coupling approximation, $N = 3$, for the scattering of positrons from atomic hydrogen.

II. DERIVATION OF THE CROSS SECTION

The usual way to solve the system of coupled equations in $F_n(\underline{r})$ is to use the method of partial waves:⁽⁶⁾

$$F_n(\underline{r}) = \sum_{\ell=0}^{\infty} \frac{f_{\ell}^{(n)}(r)}{r} P_{\ell}(\cos \theta) \quad . \quad (\text{II.1})$$

The resulting infinite number of systems of coupled equations (N coupled equations in each system) must then be solved until the contributions of the higher ℓ terms to Q_{tn} become insignificant. From Eq. (I.1), the boundary condition to be imposed upon the $f_{\ell}^{(n)}$ is:

$$f_{\ell}^{(n)}(r) \sim \frac{i^{\ell}(2\ell+1)}{k_n} \sin \left(k_n r - \frac{\ell\pi}{2} \right) \delta_{tn} + a_{tn}^{\ell} e^{ik_n r} \quad , \quad (\text{II.2})$$

where

$$g_{tn}(\theta, \phi) \equiv \sum_{\ell=0}^{\infty} a_{tn}^{\ell} P_{\ell}(\cos \theta) \quad . \quad (\text{II.3})$$

From an examination of the form of the coupled equation it is seen that if the potential terms go to zero faster than $1/r$, as r tends to infinity, then the solutions of the equations have the asymptotic form:

$$f_{\ell}^{(n)}(r) \sim A_{\ell}^{(n)} \sin\left(k_n r - \frac{\ell\pi}{2} + \lambda_{\ell}^n\right). \quad (\text{II.4})$$

If there are N coupled equations, then there exist N linearly independent solutions to the system, which must be combined with arbitrary coefficients, u_m say, to give the desired asymptotic boundary condition. For a given ℓ ,

$$\sum_{m=1}^N u_m A_m^j \sin\left(k_j r - \frac{\ell\pi}{2} + \lambda_m^j\right) = \frac{i^{\ell}(2\ell+1)}{k_j} \sin\left(k_j r - \frac{\ell\pi}{2}\right) \delta_{tj} + \alpha_{tj} e^{ik_j r}, \quad (\text{II.5})$$

where λ , the phase shifts, and A , the amplitude parameters, must be obtained from a numerical integration of the coupled equations, while δ_{tj} is the Krönecker delta. Substituting Eq. (II.3) into (I.2) yields

$$\frac{Q_{tn}}{\pi a_0^2} = \frac{4k_n}{k_t a_0^2} \sum_{\ell=0}^{\infty} |\alpha_{tn}^{\ell}|^2 / (2\ell+1). \quad (\text{II.6})$$

Equation of the coefficients of $\sin\left(k_j r - \frac{\ell\pi}{2}\right)$ and $\cos\left(k_j r - \frac{\ell\pi}{2}\right)$ in Eq. (II.5) gives the following matrix equations:

$$C \underline{u} - iD \underline{\alpha} = \underline{a} \quad (\text{II.7})$$

$$S \underline{u} - D \underline{\alpha} = 0, \quad (\text{II.8})$$

where

$$C \equiv \left(A_m^j \cos \lambda_m^j \right),$$

$$S \equiv \left(A_m^j \sin \lambda_m^j \right),$$

$$D \equiv e^{i\ell\pi/2} I \quad \text{and}$$

$$\underline{a} \equiv \frac{i^{\ell}(2\ell+1)}{k_j} (\delta_{jt})$$

Eliminating $\underline{u}$ from Eqs. (II.7) and (II.8) gives:

$$[C S^{-1} D - iD] \underline{\alpha} = \underline{a} \quad , \quad (\text{II.9})$$

where SC^{-1} is the real, symmetric derivative matrix of Wigner and Eisenbud.⁽⁷⁾ Hence,

$$\underline{\alpha}\underline{\alpha}^+ = \left(\frac{2\ell + 1}{k_t} \right)^2 [CS^{-1} - i]^{-1} E [CS^{-1} + i]^{-1T} \quad , \quad (\text{II.10})$$

where E is the operator which is unity in the tt element and zero everywhere else. Since only single-entrance channels are being considered, only the diagonal elements of $\underline{\alpha}\underline{\alpha}^+$ are required for a given t .

III. FORTRAN PROGRAM ANALYSIS

Since it is sufficient to calculate the diagonal elements of $\underline{\alpha}\underline{\alpha}^+$, we must examine which products of the elements of

$$A_{ij} \equiv (-i CS^{-1} - I)_{ij}^{-1} \quad (\text{III.1})$$

and

$$B_{ij} \equiv (i CS^{-1} - I)_{ij}^{-1T} \quad (\text{III.2})$$

are required. We see that the required products are

$$A_{ij} \cdot B_{ij}^T \quad . \quad (\text{III.3})$$

If there is defined the matrix

$$K \equiv CS^{-1} \quad , \quad (\text{III.4})$$

then the complex matrices A and B can be rewritten as

$$A_{ij} = [(-K^2 - I)^{-1} (-iK + I)]_{ij}$$

and

$$B_{ij}^T = [(-K^2 - I)^{-1} (iK + I)]_{ij} \quad .$$

Thus the complex nature of the matrices has been taken outside the inverse and is therefore much easier to work with on a computing machine.

Defining the elements of matrices as

$$x_{ij} \equiv [(-K^2 - I)^{-1} K]_{ij} \quad (\text{III.5})$$

and

$$y_{ij} \equiv [(-K^2 - I)^{-1}]_{ij} \quad , \quad (\text{III.6})$$

it is seen that

$$A_{ij} B_{ij}^T = x_{ij}^2 + y_{ij}^2 \quad . \quad (\text{III.7})$$

Substitution of the elements of Eq. (II.10) and Eq. (III.7) into the expression for the cross section, Eq. (II.6), gives

$$\frac{Q_{ji}}{\pi a_0^2} = \frac{4(k_i a_0)}{(k_j a_0)^3} \sum_{\ell=0}^{\infty} (2\ell + 1) (x_{ij}^2 + y_{ij}^2) \quad . \quad (\text{III.8})$$

A check on the results is provided by the reciprocity relation

$$k_j^2 Q_{ji} = k_i^2 Q_{ij} \quad . \quad (\text{III.9})$$

IV. EXAMPLE

For $N = 3$, we can write the first of the three linearly independent solutions as

$$\begin{pmatrix} A_{11} \sin(k_1 r - \ell\pi/2 + \lambda_{11}) \\ A_{21} \sin(k_2 r - \ell\pi/2 + \lambda_{21}) \\ A_{31} \sin(k_3 r - \ell\pi/2 + \lambda_{31}) \end{pmatrix}$$

In the following program, the parameters of each independent solution are read into the machine separately, together with the wave number of the incident particle, AC, and the partial wave under consideration, EL. The phase shifts are assigned to the locations DEL(I, J), the ℓ sum of the cross sections for a

given AC is stored in SQ, and the reciprocity values are stored in AQ. The program is established to handle up to $N = 5$, although the read and write statements for the input data would have to be modified for $N > 3$.

The matrix inversion routine used was that of Garbow.⁽³⁾

```

2  FORMAT(/26H      TOTAL CROSS SECTIONS)
4  FORMAT(/72H      KA  L  1/A11  1/A21  1/A31  D11
X      D21      D31)
54  FORMAT(F7.3,F3.0,6F10.5)
55  FORMAT(6H      F7.3,F3.0,6F10.5)
25  FORMAT(/5H      ,I2,3H  ,I2,2H  ,3F10.5)
36  FORMAT(/44H      I      J  XSEC(I,J)  SQ(I,J)  AQ(I,J))
      DIMENSION A(5,5),DFL(5,5),SQ(5,5),C(5,5),S(20,5),FK(5,5),FKK(20,5)
      1,AA(5,5),XSFC(5,5),RR(5,5),R(5,5),Z(5),AQ(5,5)
21  READ54,AC,FL,A(1,1),A(2,1),A(3,1),DEL(1,1),DEL(2,1),DEL(3,1)
      READ54,AC,EL,A(1,2),A(2,2),A(3,2),DEL(1,2),DEL(2,2),DEL(3,2)
      READ54,AC,EL,A(1,3),A(2,3),A(3,3),DEL(1,3),DEL(2,3),DEL(3,3)
      IF(AO-AC)23,31,23
23  AO=AC
      N=3.
      DO25I=1,N
      DO25J=1,N
25  SQ(I,J)=0.
      WRITE OUTPUT TAPE 3,1
      WRITE OUTPUT TAPE 3,2
31  DO5I=1,N
      DO5J=1,N
      C(I,J)=A(I,J)*COSF(DFL(I,J))
5  S(I,J)=A(I,J)*SINF(DEL(I,J))
      CALL MATINV(S,N,R,0,DETERM)
      WRITE OUTPUT TAPE 3,4
      WRITE OUTPUT TAPE 3,55,AC,EL,A(1,1),A(2,1),A(3,1),DFL(1,1),DEL(2,1
1),DEL(3,1)
      WRITE OUTPUT TAPE 3,55,AC,FL,A(1,2),A(2,2),A(3,2),DFL(1,2),DEL(2,2
1),DEL(3,2)
      WRITE OUTPUT TAPE 3,55,AC,EL,A(1,3),A(2,3),A(3,3),DFL(1,3),DEL(2,3
1),DEL(3,3)
      WRITE OUTPUT TAPE 3,36
      DO8I=1,N
      DO8J=1,N
      FS=0.
      DO7K=1,N
7  FS=FS+C(I,K)*S(K,J)
8  FK(I,J)=FS
      DO10I=1,N
      DO10J=1,N
      FS=0.
      DO9K=1,N
9  FS=FS+FK(I,K)*FK(K,J)
10  FKK(I,J)=-FS
      DO11I=1,N
11  FKK(I,I)=FKK(I,I)-1.
      CALL MATINV(FKK,N,R,0,DETFR)
      DO15I=1,N
      DO15J=1,N
      FS=0.
      DO14K=1,N
14  FS=FS+FKK(I,K)*FK(K,J)
15  R(I,J)=FS
      DO16I=1,N
      DO16J=1,N
16  PR(I,J)=R(I,J)*S(I,J)

```

```

DO17I=1,N
DO17J=1,N
17 AA(I,J)=FKK(I,J)*FKK(I,J)
Z(1) = AC
Z(2) = SQRTF(AC*AC - .75)
Z(3)=SQRTF(AC*AC-.888889)
DO20J=1,N
DO20I=1,N
XSEC(I,J)=AA(I,J)+BB(I,J)
XSEC(I,J)=((2.*EL+1.)*4.*Z(I)*XSEC(I,J))/(Z(J))**3.
SQ(I,J)=SQ(I,J)+XSEC(I,J)
IF(I-J)??,20,22
22 AQ(I,J)=XSEC(I,J)*Z(J)*Z(J)
20 WRITE OUTPUT TAPE 3,35,I,J,XSEC(I,J),SQ(I,J),AQ(I,J)
GO TO 21
END(0,0,0,0,1)

```

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TOTAL CROSS SECTIONS

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
1.200	0.	0.51271	-0.90803	-2.59555	-0.47520	-1.71347	-0.15594
1.200	0.	-1.69359	0.12454	-0.23160	-2.04030	-1.57006	-3.02570
1.200	0.	-31.24250	-0.28352	0.05808	-1.03068	-5.57229	-2.59752

I	J	XSEC(I,J)	SG(I,J)	AG(I,J)
---	---	-----------	---------	---------

1	1	0.48630	0.48630	0.
---	---	---------	---------	----

2	1	0.01887	0.01887	0.02718
---	---	---------	---------	---------

3	1	0.00085	0.00085	0.00123
---	---	---------	---------	---------

1	2	0.03941	0.03941	0.02719
---	---	---------	---------	---------

2	2	5.21279	5.21279	0.
---	---	---------	---------	----

3	2	0.22195	0.22195	0.15314
---	---	---------	---------	---------

1	3	0.00223	0.00223	0.00123
---	---	---------	---------	---------

2	3	0.27792	0.27792	0.15317
---	---	---------	---------	---------

3	3	1.71709	1.71709	0.
---	---	---------	---------	----

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
1.200	1.	1.28900	-2.42279	-7.02048	-0.12658	-0.52774	0.78886
1.200	1.	-5.24537	0.24571	-0.47511	-1.28443	-0.84540	-2.15070
1.200	1.	-109.95732	-0.58809	0.18852	-0.27815	-2.50017	-1.74932

I	J	XSEC(I,J)	SG(I,J)	AG(I,J)
---	---	-----------	---------	---------

1	1	0.58561	0.57611	0.
---	---	---------	---------	----

2	1	0.02048	0.03935	0.02949
---	---	---------	---------	---------

3	1	0.00074	0.00159	0.00107
---	---	---------	---------	---------

1	2	0.04288	0.08226	0.02959
---	---	---------	---------	---------

2	2	7.64292	12.85571	0.
---	---	---------	----------	----

3	2	0.58070	0.80265	0.40069
---	---	---------	---------	---------

1	3	0.00196	0.00419	0.00168
---	---	---------	---------	---------

2	3	0.72025	0.99617	0.35694
---	---	---------	---------	---------

3	3	19.61351	21.33060	0.
---	---	----------	----------	----

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
1.200	2.	0.16824	-0.33212	-0.95322	-0.03505	-0.49805	1.39175
1.200	2.	-0.90525	0.02512	-0.04813	-0.81443	-0.47109	-1.57977
1.200	2.	-21.99284	-0.06246	0.00957	0.21205	-1.90605	-1.24093

I	J	XSEC(I,J)	SG(I,J)	AG(I,J)
---	---	-----------	---------	---------

1	1	0.00874	0.58485	0.
2	1	0.00737	0.04672	0.01062
3	1	0.00023	0.00182	0.00033
1	2	0.01555	0.09783	0.01073
2	2	4.08870	16.94441	0.
3	2	0.75010	1.55276	0.51757
1	3	0.00051	0.00470	0.00028
2	3	0.90018	1.89835	0.49810
3	3	30.78255	52.11314	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
1.200	3.	0.01801	-0.03556	-0.10286	-0.00989	-0.25937	1.84859
1.200	3.	-0.12968	0.00209	-0.00399	-0.50146	-0.26005	-1.15412
1.200	3.	-3.75516	-0.00550	0.00070	0.53899	-1.45903	-0.89985

I	J	XSEC(I,J)	SW(I,J)	AQ(I,J)
1	1	0.00070	0.58555	0.
2	1	0.00165	0.04637	0.01258
3	1	0.00013	0.00185	0.00004
1	2	0.00344	0.10127	0.00237
2	2	1.55375	18.48190	0.
3	2	0.53665	2.15739	0.45928
1	3	0.00017	0.00477	0.00004
2	3	0.81833	2.70000	0.44348
3	3	29.52870	52.04185	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
1.200	4.	0.17380	-0.32650	-0.78631	-0.00287	-0.13035	2.22854
1.200	4.	-1.67568	0.01503	-0.03016	-0.29472	-0.13971	-0.83510
1.200	4.	-59.66452	-0.04475	0.00459	0.72015	-1.10470	-0.65171

I	J	XSEC(I,J)	SW(I,J)	AQ(I,J)
1	1	0.00005	0.58560	0.
2	1	0.00025	0.04862	0.00036
3	1	0.00044	0.00229	0.00003
1	2	0.00056	0.10183	0.00039
2	2	0.46980	18.95170	0.
3	2	0.43459	2.62395	0.29907
1	3	0.00011	0.00478	0.00000

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TOTAL CROSS SECTIONS

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	0.	1.04400	-5.51335	-44.11596	-0.51147	-1.96541	-0.70607
2.000	0.	-6.37164	0.69570	-3.90793	-2.15068	-1.29692	-2.84445
2.000	0.	-134.69093	-4.07606	0.62068	-1.48187	-2.99317	-1.79060

I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)
1	1	0.22047	0.22047	0.
2	1	0.01225	0.01225	0.04902
3	1	0.00029	0.00029	0.00115
1	2	0.01506	0.01506	0.04902
2	2	1.05448	1.05448	0.
3	2	0.02674	0.02674	0.08692
1	3	0.00037	0.00037	0.00115
2	3	0.02794	0.02794	0.08693
3	3	1.16634	1.16634	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	1.	0.16594	-1.04501	-8.67403	-0.19118	-1.34116	-0.02673
2.000	1.	-1.27296	0.10596	-0.62166	-1.54242	-0.62786	-2.28650
2.000	1.	-29.11111	-0.65324	0.09121	-0.66322	-2.45026	-1.29229

I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)
1	1	0.09354	0.31401	0.
2	1	0.02100	0.03325	0.06396
3	1	0.00042	0.00071	0.00170
1	2	0.02584	0.04092	0.08397
2	2	1.84827	2.90275	0.
3	2	0.06981	0.09655	0.22688
1	3	0.00054	0.00092	0.00169
2	3	0.07273	0.10067	0.22628
3	3	3.43136	4.59971	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	2.	0.01948	-0.11696	-0.99325	-0.07843	-0.95105	0.42886
2.000	2.	-0.15165	0.00959	-0.05752	-1.14919	-0.56615	-1.95746
2.000	2.	-3.73472	-0.06074	0.00792	-0.49429	-2.12748	-1.02862

I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)
---	---	-----------	---------	---------

1	1	0.02422	0.33823	0.
2	1	0.01664	0.04989	0.06657
3	1	0.00030	0.00101	0.00119
1	2	0.02044	0.06136	0.06643
2	2	1.72814	4.63090	0.
3	2	0.10310	0.19965	0.33506
1	3	0.00038	0.00129	0.00118
2	3	0.10736	0.20803	0.33401
3	3	4.55747	9.15718	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	3.	1.71214	-11.16344	-96.40637	-0.03297	-0.67698	0.77708
2.000	3.	-15.50904	0.74073	-4.52920	-0.05937	-0.42892	-1.71423
2.000	3.	-410.69673	-4.80264	0.59112	-0.20770	-1.88697	-0.85270

I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)
1	1	0.00536	0.34359	0.
2	1	0.00960	0.05949	0.03840
3	1	0.00015	0.00116	0.00061
1	2	0.01182	0.07318	0.03842
2	2	1.35329	5.98419	0.
3	2	0.12872	0.32837	0.41833
1	3	0.00019	0.00149	0.00060
2	3	0.13361	0.34164	0.41567
3	3	4.93830	14.09547	0.

KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	4.	0.13734	-0.98094	-8.61431	-0.01399	-0.47840	1.05960
2.000	4.	-1.47294	0.05442	-0.33023	-0.63694	-0.31680	-1.50905
2.000	4.	-41.98952	-0.35209	0.04112	0.00830	-1.68498	-0.72208

I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)
1	1	0.00109	0.34468	0.
2	1	0.00458	0.06407	0.01831
3	1	0.00006	0.00123	0.00025
1	2	0.00563	0.07881	0.01829
2	2	0.95974	6.94393	0.
3	2	0.14439	0.47276	0.46927
1	3	0.00008	0.00157	0.00025

2	3	0.15145	0.49309	0.47119			
3	3	4.89452	18.98999	0.			
KA	L	1/A11	1/A21	1/A31	D11	D21	D31
2.000	5.	0.00104	-0.00815	-0.07320	-0.00598	-0.33435	1.29680
2.000	5.	-0.01336	0.00038	-0.00231	-0.46486	-0.23380	-1.33210
2.000	5.	-0.41136	-0.00248	0.00027	0.16526	-1.49494	-0.61943
I	J	XSEC(I,J)	SQ(I,J)	AQ(I,J)			
1	1	0.00021	0.34489	0.			
2	1	0.00190	0.06597	0.00760			
3	1	0.00002	0.00125	0.00009			
1	2	0.00236	0.08117	0.00767			
2	2	0.63486	7.57679	0.			
3	2	0.15104	0.62380	0.49090			
1	3	0.00003	0.00160	0.00009			
2	3	0.15323	0.64632	0.47671			
3	3	4.61793	23.60792	0.			

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