

2009:April

English version of user manual of hctak. User and service manual, in Japanese, can be referenced to have better knowledge of the program.

HCTAK is a Continuum Discretized Coupled Channels (CDCC) program designed for heavy ion induced reactions. Formal description of CDCC is fully spelled out in the Progress of Theoretical Physics Supplement **89**(1986), which is referred as PTP in this manuscript. Spin dependent part of the optical potential is NOT accepted in the hctak. Spin orbit interaction in the projectile, however, is accepted.

Some FORTRAN programs are given.

hctak calculates S matrix elements of the CDCC.

elx uses this S matrix elements and calculates elastic scattering.

trix uses this S matrix elements and calculates triple differential cross sections.

opm calculates elastic scattering cross sections for given central potential.

wsf calculates bound and scattering state wave functions under real central potential. Fourier transform of the bound state wave function can be made. It can look for resonant states.

Those who are not familiar with numerical aspect of nuclear reactions are advised to use opm first and study the parameter dependence of the output.

Program opm may be used before adopting optical potential parameters.

Use wsf to confirm the bound state and scattering state wave functions.

Programs elx and trix can be used to calculate elastic and triple scattering cross section of CDCC.

The user is encouraged to send the questions and proposals to the author, whose e-mail address is `yaoki@tac.tsukuba.ac.jp`.

It is a great pleasure of Y. Aoki to express sincere thanks to two persons, who prepared and maintained the computational environment.

N. Okumura: Assistant Prof. Nagano Nat'l College of Technology

H. Kimura: technical staff of UTTAC

hctak is written in FORTRAN 90. It uses standard IO files of ‘hctak.in’ and ‘hctak.out’, whose logical unit numbers(lun) are 5 and 6. It writes S matrix elements onto ‘hctksmat’, whose logical unit number is 7. It refers ‘umtab’ file, on which some nuclear information such as atomic numbers, mass numbers, masses and spins are written. These files are formatted and can be handled by any editor programs. Matrix elements, (2.22c) of Chapter III of PTP, may be dumped onto ‘FFDUMP’ file, which is an unformatted file. Following table list all the files used in hctak.

file name	lun	form	main use
hctak.f			source program
tt.c			source program
hctak.in	5	formatted	standard input
hctak.out	6	formatted	standard output
hctksmat	7	formatted	S matrix output
umtab	8	formatted	nuclear database
FFDUMP	9	unformatted	matrix elements

The files ‘hctak.in’ and ‘umtab’ should be located in the same directory. If ‘hctak.out’, ‘hctksmat’ and ‘FFDUMP’ are present, hctak overwrite the calculated result, which means the old contents are lost. If they are not present, they are newly created.

building hctak

First of all, you should make an object file of tt.o by compiling tt.c. If c compiler gcc is available you can issue a command as follows.

```
|prompt > gcc -c -o tt.o tt.c
```

You can make an executable file by using a FORTRAN90 compiler and by issuing the following command to the command interpreter as,

```
|prompt > frt -O -o hctak hctak.f tt.o
```

‘frt’ of the line invokes FORTRAN compiler and the rest of the line are compiler options. ‘-O’ to optimize, ‘-o hctak’ to name the executable file to be “hctak”, ‘hctak.f’ to specify the file name of the source program and the file ‘tt.o’ be linked to the object program.

It may worth trying to ‘improve’ by invoking improve/optimize options of your FORTRAN compiler.

use of MPI

If available, you can use message passing interface (MPI) option. You should activate some commented-out lines in the source program, which are sandwiched by the lines, which begins with ‘C MPI’.

To secure output process, every CPU use their own standard and S matrix files when

MPI is used. They are named as ‘hco?????’ and ‘smt?????’, where ‘?????’ stands for the ID number of each CPU with leading zeros padded.

CDCC equations(PTP III 2.16) with different J, the total angular momentum of the system, are solved on separate CPU’s. It is recommended to prepare the matrix elements(PTP III 2.22c) on ‘FFDUMP’ before using MPI.

Input data

Input data consists of some readable lines, which contain less than 80 characters. Leading two lines are read with the fixed format, while rest of the lines are free format under FORTRAN rule. You can follow the examples given later.

0-th group TITLE with (A50) format

This line is intended as a column indicator and I use as follow,

```
2   4   6   8  10      | title begins
```

This line has no further meaning at all.

1st group (KNTL(i, i = 1, 10),TITLE with (10I2,5X,A50) format

KNTL(1) spin coupling scheme

=-1: reset intrinsic spins of particles 1, 2 and 3, i.e., $s_1 = s_2 = s_3 = 0$.

= 0: $\mathbf{s}_1 + \mathbf{s}_2 = \mathbf{s}$, $\mathbf{l} + \mathbf{s} = \mathbf{I}$

=1: $\mathbf{l} + \mathbf{s}_1 = \mathbf{j}$, $\mathbf{j} + \mathbf{s}_2 = \mathbf{I}$

=9: Read parameters of particles 1, 2 and 3.

KNTL(2) NLSJ: number of different spin states. max. of 15.

KNTL(3) Handling Coulomb potential of V_{12} and V_{13}

=0: No Coulomb break up.

=1: Coulomb break up is taken into account.

=2: Include Uehling potential between center of masses of (1+2)-3 system.

=3: Coulomb break up with Uehling potential

KNTL(4) print radial part of Φ , (PTP III 2.10c)

=n ($n > 0$): print every n step.

=-n($n > 0$): print overlap integrals (PTP III 2.11) only.

KNTL(5) If positive, print V_{12} and V_{13} every KNTL(5) step.

KNTL(6) If positive, print matrix elements (PTP III 2.22c) every KNTL(6) step.

KNTL(7) If positive, print coupling matrix elements (PTP III 2.22a) every KNTL(7) step. Actually output includes kinetic energy, so $(V - E)_{c'c}$ in unit of MeV with no centrifugal potential.

KNTL(8) Dump/read matrix elements (PTP III 2.22c) onto/from FFDUMP.

=1: Dump matrix elements then continue the calculation.

=2: Read matrix elements and solve CDCC equation.

KNTL(9) Print S matrix elements.

=1: print onto standard output.

=2: print onto S matrix file.

=3: both.

$1/\sqrt{\Delta k}$ (PTP III 2.19b) are multiplied to the S matrix elements of the break up channel.

KNTL(10) Reserved.

TITLE Write reaction and incident energy like,

(p+22Mg)+12C, E(A1)=1840 MeV

hctak read each character and identifies as you may intended. For this example, incident particle consists of a proton and magnesium 22. Target is carbon 12. Incident energy of aluminum 23 is 1840 MeV.

In this case, particle 1 (2) is a proton (^{22}Mg) and particle 3 is a ^{12}C . You are advised NOT to fool hctak, because the program is not clever enough.

Place 3 lines here when KNTL(1)=9.

1-2, 1-3 (IZ(I), IA(I), IS(I), JP(I), EM(I), I = 1, 2)

I=1 and 2 correspond to particles 1 and 2, respectively.

IZ atomic number of particle I.

IA mass number of particle I.

IS twice the spin of particle I, in $[\hbar]$.

JP parity of particle I.

EM mass of particle I in atomic mass unit, i.e., that of electrically neutral atom having ^{12}C as its nucleus is 12 exact.

1-4 IZ(3), IA(3), IS(3), JP(3), EM(3), ELAB

Particle parameters of particle 3.

ELAB is the kinetic energy of incident particle, bound state of particles 1 and 2, in MeV.

blank line This line is placed to keep visibility of the input data.

Rest(2-1 group to the last) of the input lines are format free.

The lines named 2-1 to 2-4 specify internal structure of the system 1-2 and index 'N' of the variables run from 1 to NLSJ,(=KNTL(2)). NLSJ sets of this data group should be given.

2-1 group LSTAB(N), ISTAB(N), JSTAB(N), NBND(N), NRES(N), IDVS(N)

LSTAB(N) l of N-th spin state of 1-2 system, (PTP III 2.7a)

ISTAB(N) s of N-th spin state of 1-2 system, (PTP III 2.7a) if KNTL(1)=0,
and j if KNTL(1)=1

JSTAB(N) I of (PTP III 2.7a)

NBND(N) Number of bound states in N -th spin state.

NRES(N) Number of resonant states in N-th spin state.

IDVS(N) Potential ID, which is used to generate radial wave functions of N-th spin state.

2-2 group (NODS(I), ISBE(I), BES(I), I= 1, NBND(N))

This line specifies bound state nature and is necessary only when NBND(N) is a positive integer and should not be input otherwise.

NODS(I) Number of nodes, which does not include the ones at zero and at infinity.

ISBE(I) Specify binding energy or potential depth to be kept.

=0: adjust depths of the ‘floating potential’ to reproduce given binding energy.

=1: adjust binding energy to calculate bound state wave function.

BES(I) Binding energy in MeV. You are advised to give a proper binding energy even if ISBE(I)=1. You can use separate program ‘wsf’ for this purpose.

Maximum number is limited as $\sum_N \sum_I NODS(I) < 11$.

2-3 group (FKR(I), WKR(I), I= 1, NRES(N))

FKR(I) Resonant wave number in fm^{-1} .

WKR(I) Integration width of the resonant state in fm^{-1} .

These resonance information lines should be placed in NRES(N) lines and should never be given if $NRES(N) \leq 0$.

Variables FKR and WKR specify the integration range (PTP III 2.10c) as follow,

$$\Phi_c = \int_{k_{i-1}}^{k_-} dk + \int_{k_-}^{k_+} dk + \int_{k_+}^{k_i} dk(\dots), \quad (1)$$

where $k_{\pm} \equiv FKR(I) \pm WKR(I)$, i.e., resonant region is integrated carefully.

You can use ‘wsf.f’ program to check the presence/absence and parameters of resonant states.

2-4 group NKSBIN(N), FKSMIN(N), FKSMAX(N)

These variables specify the integration range of (PTP III 2.10c), NKSBIN is the number of k-bins, FKSMIN and FKSMAX set the minimum and the maximum of wave numbers in fm^{-1} .

3rd group NVPS, NR12, DR12, LAMMIN, LAMMAX

NVPS Number of independent potentials for 1-2 system. In principle this should be unity to guarantee (PTP III 2.11).

NR12, DR12 Number and size of radial variable ρ meshes in 1-2 system. Default value is used if NR12=0.

LAMMIN, LAMMAX Range of λ in (PTP III 2.21). LAMMIN is reset to 0 even if positive integer is given, to ensure diagonal matrix elements be given to solve CDCC equation correctly.

4-th group (((VPS(J, I, N), J= 1, 6), I= 1, m), N= 1, NVPS)

This group define potential parameters of 1-2 system. ‘m’ should be less than or equal to 5. Maximum of six parameters are given in each line, so number of this

input lines are $\sum_{N=1}^{NVPS} m$. NVPS is defined in the [3rd group].

Potentials defined by using 'm' lines are superposed and form a set of 1-2 potential.

VPS(1,?,?) Controller of potential attribute.

=±1 if this line defines the fixed potential

=±2 if this line defines the floating potential, i.e., potential depth is adjusted to reproduce the given binding energy.

Negative or zero value of VPS(1,?,?) specifies to terminate this line scan for fixed 'N'. The line next to this negative or zero VPS(1,?,?) specifies the beginning of next set of (1-2) potential or transit to 5-th group.

VPS(2,?,?) define potential type

=1: Volume type potential, $V/(1+e)$

=2: Surface type potential, $4Ve/(1+e)^2$

=3: Modified Thomas-Fermi type, $2V(\mathbf{l} \cdot \mathbf{s})e/(1+e)^2$

where $e \equiv \exp((r-R)/a)$. 'V', 'R' and 'a' are define below.

VPS(3-5,?,?) 'V', 'R', and 'a' in this order of the potential type in MeV or in fm.

Notice radius parameter is NOT scaled by $A^{1/3}$ nor $A_1^{1/3} + A_2^{1/3}$.

V should be negative for attractive or absorptive potential.

VPS(6,?,?) Coulomb charge radius R_C in fm. This charge radius should be given only once for each NVPS set of input.

$$V_C(\rho) = \frac{z_1 z_2 e^2}{4\pi\epsilon_0} \begin{cases} \frac{1}{2R_C} \left\{ 3 - \left(\frac{\rho}{R_C} \right)^2 \right\} & \text{if } \rho \leq R_C \\ \frac{1}{\rho} & \text{otherwise} \end{cases} \quad (2)$$

blank line You may write any comment here.

Now follows the data to specify (1+2)-3 system.

5-th group (VPL(J, I, N), J = 1, 6)

These lines define optical potential of particle N(= 1 or 2) and particle 3. Maximum number of I in the above expression is 10. Potentials with different I and same N are superposed to define particle N-particle 3 optical potential.

VPL(1,?,?) Specify real or imaginary part.

= ±1 for real part.

= ±2 for imaginary part.

Negative or zero VPL(1,?,N) indicates the end of potential set of N-th particle.

VPL(2,?,?) Define functional form. Definition of the potential type is the same for (1-2) potential.

=1: Volume type

=2: Surface type

VPL(3-5,?,?) in this order are V , R , a of the potential in MeV or in fm.

VPL(6,?,?) Coulomb charge radius(R_C) in fm. This parameter should be given only once in any of the 'I' lines.

6-th group NRF, (DRF(M), RF(M), M= 1, NRF)

Table of matrix elements (PPT III 2.22c) are stored as a function of R . This line defines this R table and is interpreted as follows. Mesh size of R from $R = 0$ to $R=RF(1)$ is DRF(1), from $R = RF(i-1)$ to $RF(i)$ mesh size is DRF(i-1). If we write part of the R table explicitly it looks like, $R = 0$, DRF(1), 2 DRF(1), \dots , $RF(1)$, $RF(1)+DRF(2)$, $RF(1)+2 DRF(2)$, \dots , $R=RF(NRF)$.

Maximum R table size is 300.

Matrix elements at any R are interpolated by using 3rd order spline. You don't need to keep DRF very small, where matrix elements are expected to change gradually.

CDCC equation is integrated from $R = 0$ to $RF(NRF)$ with a step size of DR3, which is given in the next line.

7-th group JTMIN, JTMAX, JTINC, DR3

JTMIN Twice the minimum number of J (PTP III 2.7a) in \hbar .

JTMAX Twice the maximum of J.

JTINC Increment of twice J.

DR3 Step size in integrating CDCC equation(PTP III 2.16) in fm.

Notice JTMIN and JTINC should be given according to the angular momentum rule. If the spin $s = 1/2$ and you give JTMIN=0, hctak will give you an error message and abort.

The **7-th group** is the last input to hctak.

Sample Input

Following 22 lines show a sample input of $^{58}\text{Ni}(d,d)$ reaction. Parameters are taken from (PTP III Table I).

```

  2   4   6   8  10           column identifier
0 4 0 0 0 0 0 0 2 0         (p+n)+58Ni, Ed=56 MeV
---- system 1-2 ----
0 2 2 1 0 1 /LSTAB, ISTAB, JSTAB, NBND, Nres IDVS: Gnd, 3S1 state
0 0 2.22      /NODS, ISBE, BES: depth adjust
4 0.0 1.0      /NKSBIN FKSMIN FKSMAX
2 2 2 0 0 1 /LSTAB, ISTAB, JSTAB, NBND, Nres IDVS: 3D1 state
4 0.0 1.0      /NKSBIN FKSMIN FKSMAX
2 2 4 0 0 1 /LSTAB, ISTAB, JSTAB, NBND, Nres IDVS: 3D2 state
4 0.0 1.0      /NKSBIN FKSMIN FKSMAX
2 2 6 0 0 1 /LSTAB, ISTAB, JSTAB, NBND, Nres IDVS: 3D3 state

```

```

4  0.0 1.0      /NKSBIN FKSMIN FKSMAX
1  0 0.1 0 6 /NVPS, NR12, DR12, Lammin, Lammax
-2 1 -27.8655  2.4  0.65 2.4/VPS(1-6)
---- sys. 1/2-3  Watson,(??) pot. ----
1  1 -48.76  4.53 0.75    5.03 /VPL(*,1,1)
2  1  -3.460 5.11 0.5341  0.0  /VPL(*,2,1)
-2 2  -5.214 5.11 0.5341  0.0  /VPL(*,3,1)
1  1 -46.51  4.53 0.75    4.84 /VPL(*,1,2)
2  1  -4.60  4.88 0.58    0.0  /VPL(*,2,2)
2  2  -5.586 4.88 0.58    0.0  /VPL(*,3,2)
0    /potential 2-3 terminator
1  0.5 30.0 1.0 40.0  2.0 100.0 10.0 1000/NRF,(DRF(i),RF(i),i=1,NRF)
0  100  2    0.05D0/ JTmin, JTmax, JTinc, DR3
+++++
C  KNTL(1): =-1 reset spins
C           =0 for LS:
C           =1 for jj coupling
C  KNTL(2): number of indep. spin states NLSJ
C  KNTL(3): Coulomb ex. and vacuum pol.
C  KNTL(4): sys1-2 wave functions
C  KNTL(5): V1-3 and V2-3 potential
C  KNTL(6): sys1-2 matrix elements
C  KNTL(7): coupling matrix elements
C  KNTL(8):=1 dump to FFDUMP
C           =2 read from FFDUMP
C  KNTL(9): S matrix output:=1, print, =2 file
C  KNTL(10): reserved

```

Slashes '/' in the input data dictate to terminate the input action for the READ statement. Rest of the columns are used as reminders.

The last figure 4.84 in VPL(*,1,2), neutron charge radius, may be useless.

The line which contains many '+' and below are placed just to be a reminder.

Coulomb break up option is not used in this sample input. You can use this option just by giving KNTL(3)=1. Notice, however, that the program works under your input, NOT by your intention ! The author advises the user to output and plot every stage of the calculation and think if the output really reflect the intention.

Sample Output

Part of the output file for the sample input is shown with some comments, which are sandwiched by leading '+++++' lines. The program worked as a dummy MPI mode.

+++++

Under MPI mode, hctak output the following line to indicate MPI is used

+++++

NPROCS, MYRANK, STD0, SMF= 1 0 hco00000 smt00000

date=2009/ 4/17/ 9: 1:46

hcz program version 2008/01/02 by Y. Aoki

2 4 6 8 10 title

0 4 0 0 0 0 0 2 0 (p+n)+58Ni, Ed=56 MeV

+++++

'title' of (1st group) is converted like following 5 lines.

+++++

sys	Ename	Z	A	J	pi	M[u]
1	H	1	1	1/2	+	1.0073
2	N	0	1	1/2	+	1.0087
3	NI	28	58	0	+	57.9200

Elab((1+2)-3)= 56.0000 MeV

+++++

(2nd-4-th group) input are confirmed.

+++++

***** system 1-2 in LS coupling*****

Ch	LS	2S	2J	Nbnd	Nkbin	K(min)	K(max)	Pid
1	0	2	2	1	4	0.0000	1.0000	1
2	2	2	2	0	4	0.0000	1.0000	1
3	2	2	4	0	4	0.0000	1.0000	1
4	2	2	6	0	4	0.0000	1.0000	1

bound state(s)

Ch	Node	BE	isBE?
1	0	2.2200	0

System 1-2: potential parameters

I1=1(2) fixed (floating) part I2=1(2) volume (surface) type

Pid	I1	I2	V[MeV]	R[fm]	a[fm]	RC[fm]
1	2	1	-27.86550	2.40000	0.65000	2.40000

+++++

(5-th to 7-th group) are confirmed

+++++

System 1/2-3 optical potential parameters

I1=1(2): real (imag.) part. I2=1(2) volume (surface) type

sys	I1	I2	V[MeV]	R[fm]	a[fm]	RC[fm]
1-3	1	1	-48.7600	4.53000	0.75000	5.03000
1-3	2	1	-3.4600	5.11000	0.53410	0.00000
1-3	2	2	-5.2140	5.11000	0.53410	0.00000
2-3	1	1	-46.5100	4.53000	0.75000	4.84000
2-3	2	1	-4.6000	4.88000	0.58000	0.00000
2-3	2	2	-5.5860	4.88000	0.58000	0.00000

NR12= 600 DR12= 0.1000 fm. Lambda= 0 to 6
R3=0 to 30.00 fm (DR3= 0.05000 fm)*(600 steps)
2*Jtot= 0 to 100 step 2

HCTKMS: N12= 17, NFF= 470

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***** HCTK20 entered *****

+++++

system 1-2 information is now converted

ID=1 means 3S1 state

+++++

System 1-2 ch. ID= 1

potential parameters

I1	I2	V[MeV]	R[fm]	a[fm]
2	1	-27.8655	2.4000	0.6500

+++++

bound state is solved by adjusting the floating part of the potential depth

Vfac is the scaling factor of this potential

+++++

WSBND: ISBE= 0

Loop	LS	NS	NN	Vfac	BE(MeV)	FI
0	0	0	0	1.00000	2.22000	-2.07145E-02
1	0	0	0	0.97929	2.22000	-6.37518E-04
2	0	0	0	0.97866	2.22000	-5.54605E-07

<r>= 3.7679E+00 sqrt(<r*r>)= 4.4237E+00 fm

+++++

Four scattering state wave functions are generated, because NKBIN=4,

whose ID are given to be 2 to 5. Bound state ID=1

+++++

Ch	ID	NK	k_range	delta_k	Norm**2
1	2	50	0.0000E+00 2.5000E-01	2.5000E-01	9.2195E-01
1	3	50	2.5000E-01 5.0000E-01	2.5000E-01	9.5390E-01

1	4	50	5.0000E-01	7.5000E-01	2.5000E-01	9.5298E-01
1	5	50	7.5000E-01	1.0000E+00	2.5000E-01	9.5460E-01

+++++

Now follows scattering wave calculation with modified potential depth.

+++++

System 1-2 ch. ID= 2

potential parameters

I1	I2	V[MeV]	R[fm]	a[fm]
1	1	-27.2709	2.4000	0.6500

+++++

Some lines are deleted to save space.

Then follows the table of system 1-2 information.

17 wave functions, 1 bound+4x(4 spin state of 3S1, 3D1, 3D2, 3D3)=17.

delta is a phase shift

+++++

quantum numbers of system 1-2

ID	E[MeV]	k[/fm]	Eta	N	L	2*S	2*J	delta[rad]
1	-2.22000	-0.23131	0.00000	0	0	2	2	0.00000
2	0.86445	0.14434	0.00000	-	0	2	2	2.42050

+++++ lines for ID=3 to 16 are deleted +++++

17	31.98466	0.87797	0.00000	-	2	2	6	0.28568
----	----------	---------	---------	---	---	---	---	---------

VDCAL: potential parameters

I1=1(2) real(imag.) I2=1(2) volume(surface) pot.

sys	I1	I2	VV	RR	AA	DR	Rmax
1-3	1	1	-48.7600	4.5300	0.7500	0.1875	14.8125
1-3	2	1	-3.4600	5.1100	0.5341	0.1335	12.4178
1-3	2	2	-5.2140	5.1100	0.5341	0.1335	12.4178
2-3	1	1	-46.5100	4.5300	0.7500	0.1875	14.8125
2-3	2	1	-4.6000	4.8800	0.5800	0.1450	12.9050
2-3	2	2	-5.5860	4.8800	0.5800	0.1450	12.9050

IZ(1)= 1 IZ(2)= 0 IZ(3)= 28

Rcoul(1)= 5.03 Rcoul(2)= 4.84 Rcoul((1+2)-3)= 5.03 [fm]

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***** HCTK40 entered *****

allocated memories

NCC	KCC	NZS	NRFF	ICW	NUV	NU	IFCC	sum
75	42	17	60	1080	14112	17640	220332	253803

+++++

Before going into solving CDCC equation, CDCC state[(1+2)-3] information is tabulated. One 1-2 state with spin I is split into (2I+1) CDCC states.
 $2*L_{cm} = 2(J-L)$ if we use (PTP III 2.14b) notation.

+++++

coupled channels base

ID	Ecm[MeV]	KCM[/fm]	eta	2*Lcm	L	2*S	2*I	k(1-2)[/fm]
1	54.118596	2.245346	0.836405	-2	0	2	2	-0.231305
2	51.034146	2.180422	0.861310	-2	0	2	2	0.144338

+++++ lines of ID=3 to 73 are deleted +++

74	35.474040	1.817881	1.033081	6	2	2	6	0.629153
75	19.913934	1.362036	1.378832	6	2	2	6	0.877971

+++++

Next lines confirm the status of Coul. wf calculation at the matching radius

+++++

Coul. wf: Rmatch= 29.900 fm Lmax= 53

rho	Eta	L	Wronsk.-1
6.714E+01	8.364E-01	51	8.3267E-16
6.519E+01	8.613E-01	46	5.5511E-16
6.179E+01	9.087E-01	44	8.8818E-16
5.435E+01	1.033E+00	47	7.7716E-16
4.072E+01	1.379E+00	52	2.4425E-15

***** CC stage entered *****

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+++++

CDCC equation is solved with given J and parity (Jpar).

NS0 shows where the integration started.

KCC is the number of coupled channels and Cnum is the condition number of the problem when S matrix is solved.

+++++

2*Jtot= 0 NS0= 1
 0 -1 13 1.277E+01 /JT2 Jpar KCC Cnum

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2*Jtot= 2 NS0= 1
 2 1 30 1.907E+01 /JT2 Jpar KCC Cnum
 2 -1 21 1.188E+01 /JT2 Jpar KCC Cnum

+++++ lines for Jtot=4 to 99 are deleted +++++

date=2009/ 4/17/ 9: 2: 4

2*Jtot= 100 NS0= 254
 100 1 33 5.214E+03 /JT2 Jpar KCC Cnum
 100 -1 42 2.468E+04 /JT2 Jpar KCC Cnum

MPI_FINALIZE called

S matrix file

Content of 'hctksmat', in this sample case its name is 'smt00000', looks as follows. Lines with leading '+++++' are added for explanation and are not present in the real output.

+++++

Leading 2 lines are just the leading 2 lines of the hctak input.

3rd line tells that 17 wave functions are used in describing 1-2 system, and their information follows.

+++++

```

  2   4   6   8  10           title
0 4 0 0 0 0 0 0 2 0      (p+n)+58Ni, Ed=56 MeV
 17  /N12  quantum numbers of system 1-2
ID   E[MeV]   k[/fm]   Eta    N  L  2*S  2*J   delta[rad]
 1  -2.22000 -0.23131  0.00000  0  0  2   2   0.00000
 2   0.86445  0.14434  0.00000  -  0  2   2   2.42050
+++++ states 3 to 15 are deleted +++
16  16.42456  0.62915  0.00000  -  2  2   6   0.12693
17  31.98466  0.87797  0.00000  -  2  2   6   0.28568
 75   0 100   2   0   2  /NCC JT.., LS 2*I
ID  Ecm(MeV)   Kcm[/fm]   eta    2*Lcm L  2*S  2*I  k(1-2)[/fm]
 1  54.118596  2.245346  0.836405  -2  0  2   2  -0.231305
 2  51.034146  2.180422  0.861310  -2  0  2   2   0.144338

```

+++++

17 states of 1-2 system are split into 75 CDCC states and information of this 75 CDCC states follows.

Information from 3 to 73 are deleted

+++++

```

 74  35.474040  1.817881  1.033081  6  2  2   6   0.629153
 75  19.913934  1.362036  1.378832  6  2  2   6   0.877971

```

+++++

Then follows S matrix information for each J,pi.

JT2 is twice the J, Jpar for parity, Kcc for number of coupled states for given J and parity, Cnum is a condition number and IDCC table tells coupled state ID in CDCC mode.

Inc. ch is the channel, which contains incoming wave. Rest of the channels has outgoing wave only.

|S|**2 is the square sum of the outgoing wave amplitude. It is unity if no absorption take place.

Rest of the 2*Kcc entry are S matrix elements, i.e., in essence, complex amplitude of the outgoing wave of Kcc channels.

+++++

```

    0   -1   13   1.28E+01  /JT2 Jpar Kcc Cnum IDCC follows
  11   12   13   14   15   24   25   26   27   72   73   74   75
  -1   11   1.75631E-02  /Jpar Inc. ch, |S|**2
-7.9710E-02 -3.3900E-02 -2.4413E-02 -7.5221E-02 -5.7860E-02 -8.7792E-02
 3.3473E-02  3.1400E-02 -1.9991E-02 -8.8017E-02  1.1179E-02 -1.9195E-02
-2.1753E-02  2.4124E-02 -2.1778E-02 -1.8707E-02  3.0012E-02  3.4096E-02
-1.0094E-02  2.3429E-02 -1.8939E-02 -2.1437E-02  3.6658E-02 -2.8645E-02
-6.3209E-02  2.4769E-02

```

+++++

S matrix output till JT2=JTMAX. All but the tailing two lines are deleted.

+++++

```

-1.1976E-08  3.8149E-08  1.0326E-12 -1.6602E-12 -6.6044E-06  1.6494E-05
-5.2320E-07  9.0435E-07 -1.0086E-08  3.1113E-08  3.8715E-13 -6.7416E-13

```

elx

elx.f calculate differential cross section by using a set of S matrix elements, which is an output of hctak.

elx.f can be compiled by using a FORTRAN90 compiler as,

```
|prompt> frt -o elx elx.f
```

and you will get an executable file of elx.

Input data

Program elx uses standard I/O files with logical unit numbers 5 and 6, whose file names are 'elx.in' and 'elx.out'. Input format is almost the same as hctak and is line oriented. Here is a sample input, which uses S matrix of the above sample input of hctak.

```

0 0 0 0 0  test test
0 180.0 1  /ang0, ang1, dang, JT2LIM
smt00000

```

1st group (KNTL(i), i= 1, 5), TITLE

No KNTL data is actually used.

2nd group ANG0,ANG1,DANG, JT2LIM

Leading three variables, ANG0, ANG1, DANG, define the angular range, 1st and last angles and angle increment in degree.

JT2LIM limit the maximum angular momentum even though S matrix table gives

up to $(JTMAX/2) \cdot 2 \times J_{max} = \min(JT2LIM, JTMAX)$, where JTMAX is defined in **7-th group** of hctak.

3rd group FNAME with format (A30)

File name of S matrix table, which is an output of hctak with logical unit number of 7 and named hctksmat.

Sample output

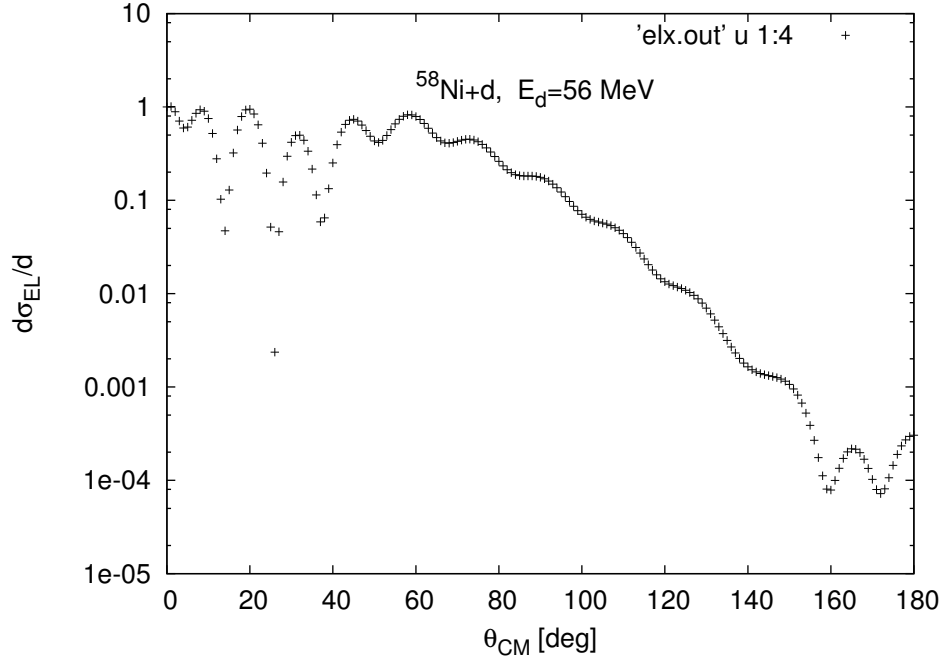
Output of elx is given below. Leading 4 lines reflect the input. 5-th line tells the column meaning. Columns 'Ang(deg)' and 'Xsec(mb/sr)' are for scattering angle in degree and differential cross $d\sigma/d\Omega$ in mb/sr in center of mass system. Columns 'Xruth' and 'Xel/Xruth' are Rutherford scattering cross section and the ratio of elastic cross section to Rutherford one. Cross section at zero degree for charged particle pair has no physical meaning, however. The line with 'tot. reac. Xsec' tells the total reaction cross section in mb.

```

prog. elx ver. 2009/01/14 by Y. Aoki
      test test
      S mat file=smt00000
      0 4 0 0 0 0 0 0 2 0      (p+n)+58Ni, Ed=56 MeV
#Ang(deg)  Xsec(mb/sr)  Xruth    Xel/Xruth
      0.000   3.4690e+39   3.4690e+39   1.0000e+00
      1.000   6.0509e+07   5.9819e+07   1.0115e+00
      2.000   3.3251e+06   3.7393e+06   8.8924e-01
+++++ lines for 3 to 178 degree are deleted +++++
      179.000  1.0255e-04   3.4695e-01   2.9557e-04
      180.000  1.0554e-04   3.4690e-01   3.0422e-04
# tot. reac. Xsec=   1.827e+03 mb

```

Following graph is a plot of column 1 vs. column 4 of the above output.



Program elx.f calculates the following quantity as scattering amplitude,

$$f_{m_f m_i} = f^C(\theta) \delta_{m_f m_i} + f_{m_f m_i}^N(\theta) \quad (3)$$

$$f_{m_f m_i}^N(\theta) = \sum_{l_i l_f j} \frac{\sqrt{4\pi}}{k} \sqrt{2l_i + 1} e^{i\sigma_{l_i}} \langle l_i 0 s m_i | j m_i \rangle \times C_{l_f l_i}^j e^{i\sigma_{l_f}} \langle l_f m s m_f | j m_i \rangle Y_{l_f m}(\hat{\mathbf{K}}_f) \quad (4)$$

where

$$f^C(\theta) = -\frac{\eta}{2k \sin^2 \theta/2} e^{-i(\eta \log \sin^2 \theta/2 + 2\sigma_0)} \quad (5)$$

is a scattering amplitude of Coulomb scattering and $\langle l m_l s \sigma | j m \rangle$ is a Clebsch-Gordan coefficient. Rest of the notation should be well known.

trix

Program trix.f calculates triple differential cross section, where particles 1 and 2 are detected in coincidence. It uses S matrix elements, which are output from hctak. It is written in FORTRAN90 and the executable file can be made as follows,

```
|prompt> frt -o trix trix.f tt.o
```

As stated in the hctak section, tt.o gives current time in unix definition and should be compiled separately.

Input and output files of the program are as follows,

file name	lun	form	main use
trix.f			source program
tt.c			source program
trix.in	5	formatted	standard input
rix.out	6	formatted	standard output
hctksmat*	7	formatted	S matrix file
umtab	8	formatted	nuclear data base

* This file name can be specified by the user.

Input data

0-th group Just a column indicator, as is hctak.

1-st group (KTRL(i), i= 1, 10), TITLE in format (10I2,A50).

KTRL(1) =1 exchange particle 1 and particle 2, i.e., particle 2 of hctak is treated as particle 1 in trix.

KTRL(2) reserved for slit information of particle 1. KTRL(2)=1 for circular, =2 for rectangular slit. These options are NOT supported yet.

KTRL(3) reserved for slit information of particle 2. Same as KTRL(2).

KTRL(4) repeat evaluation of triple differential cross section by changing scattering angles as is indicated in the following table.

KTRL(4)	angle	particle
1	polar angle	1
2	azimuthal angle	1
3	polar angle	2
4	azimuthal angle	2

KTRL(2-4) apply to the particles after 1 and 2 exchange is made, if KTRL(1)=1.

KTRL(5) reset intrinsic spins to zero.

KTRL(6) reserved for double differential cross sections.

KTRL(7) reserved for single differential cross sections.

KTRL(8) not used yet.

KTRL(9) not used yet.

KTRL(10) =1, suppresses printing triple differential cross sections for polarized projectile and ejectiles.

TITLE Any sentence may be written.

2nd group SFILE in format (A20)

One can specify S matrix file name.

No format specification is made for 3rd to last group.

3rd group QVAL, NE1, E1MN, E1MX, JT2LIM

QVAL Minus the binding energy of particle 1 and 2 in MeV.

NE1 specify number of kinetic energies of particle 1, for which triple differential cross sections are to be evaluated.

E1MN and E1MX Minimum and maximum kinetic energies of particle 1, for which triple differential cross sections are to be evaluated.

NE1, E1MN and E1MX define the kinetic energies of particle 1.

JT2LIM Set the upper limit of the total angular momentum of the whole system.

Minimum of **JTMAX**, written in the S matrix file, and **JT2LIM** is used to be twice the maximum of total angular momentum in \hbar .

4-th group (**ANG1**(i, 1), i = 1, 5)

Specify detection angles of particle 1 in degree.

ANG(1) polar angle

ANG(2) azimuthal angle

ANG(3) half the apex angle or
half the aperture angle

ANG(4) half the aperture angle

ANG(5) rotation angle

Circular or rectangular slit is assumed. These slit information, however, is not used yet.

5-th group (**ANG1**(i, 2), i = 1, 5)

Corresponding angles of particle 2 as 4-th group.

6-th group **NANG**, **ANGMIN**, **DANG**, **NTERMS**

This group is valid when **KTRL**(4) > 0 and specifies how the corresponding angle is varied while repeating the calculation. Three variables define number, 1st and increment of the scattering angle in degree.

NTERMS specify the number of quasi-random-numbers. Double differential cross section is evaluated by integration of triple differential cross section over solid angle of particle 2. This surface integration is roughly made by using good lattice points, which are generated by using consecutive two Fibonacci numbers N_0 and N_1 . Smaller one, N_0 is the smallest integer which is larger or equal to **NTERMS**.

One should not modify the content of 'hctksmat'.

Input sample

```
1 2 3 4 5 6 7 8 9 0  written here is a column indicator
1 0 0 0 0 0 0 0 0 0  here is a second title
smt00000
100  -0.125 1600.0 1840.0, 0 /NE1, Qval E1MN E1MX LT2LIM
5, 0.0, 0.0, 0.0 0.0      / ang1(1-5)
```

```

10.0, 0.0, 0.0, 0.0 0.0 / ang2(1-5)
20 2 2 /Nang, Ang0, Dang effective if KTRL(4)>0

```

S matrix file named is smt00000, which is an output from the MPI version of the hctak.
Output sample

```

Your input KTRL= 1 0 0 0 0 0 0 0 0 0
          title= here is a second title
S mat. file=smt00000          Qval= -0.1250 [MeV]

```

```

Ang(*,1):  5.00   0.00   0.00   0.00   0.00 [deg]
Ang(*,2): 10.00   0.00   0.00   0.00   0.00 [deg]
Slit(1) : - - -      Slit(2) : - - -

```

sys	Ename	Z	A	J	pi	M[u]
1	H	1	1	1/2	+	1.0073
2	MG	12	22	0	+	21.9930
3	C	6	12	0	+	11.9967

Elab((1+2)-3)= 1840.0000 MeV

```

**** particle param 1 <--> 2 ****
+++++
Intrinsic spins manipulation is NOT specified by the input, but was
specified to be so to the input of the hctak.
The program hctak write the TITLE line to the smt00000, which is
read by the program trix and the intent of the TITLE is observed here.
So the following line is output.

```

```

+++++
**** spins are set to ZERO ****

```

```

NLSJ=  5   ISJJ=  0
LS  JS  II  NK  IP
 2   0   4  26   1
 1   0   2  25  27
 0   0   0  25  52
 3   0   6  25  77
 4   0   8  25 102

```

```

+++++
Above 5 lines show how the trix read some leading lines of smt00000
+++++

```

IS1	IS2	IIO	ISN	ISX	LSMAX	IIMAX	MSMAX	MLMAX
0	0	4	0	0	4	8	4	6

NLJI	NLJK	NCM	KCMX	NG12	NG3	JTMIN	JTMAX
25	130	650	378	25	165	0	1000

Main: malloc. parameters

NS0	NS1	NS2	NE1	NLSJ	NLJI	MLMAX	LMAX	JMNX	NYL
5	1	1	100	5	25	6	504	501	3535

***** new and old NE1= 89 100 *****

TRIX0: E1 range: 1.6000E+03 1.8382E+03 step 2.382 MeV NE1= 89

P1 range: 2.4808E+03 8.6761E+03 MeV/c

S range: 2.1079E+03 3.0977E+03 MeV/c

Sp Shx Amom= 3.0977E+03 3.0748E+03 5.5785E+03 MeV/c

+++++

NE1 is specified to be 100, but is reduced to be 89, because some of the kinetic energies specified by E1MX and NE1 are not reachable.

This is so because of the kinematics or by truncation of k_{max} to be k_{max} in {\bf group 2-4} of hctak.

As for the S range to Amom, one should refer to the service manual.

+++++

#TRIX1: Triple diff. Xsec in [mb/sr**2 MeV]

+++++

The 4-th column is the triple differential cross section in mb/sr**2 MeV for the kinetic energy and momentum of columns 1 and 2.

Column 3 stands for the wave number of the 1-2 relative motion in 1/fm.

+++++

#E1(MeV)	P1 [MeV/c]	k12 [/fm]	tri_Xsec
1601.191	8.09749E+03	1.24113E+00	1.24646E-04
1603.573	8.10351E+03	1.22292E+00	1.40451E-04

+++++

More than 80 lines are deleted.

+++++

1806.052	8.59992E+03	1.41868E+00	1.42929E-04
1808.434	8.60558E+03	1.54792E+00	1.06418E-04
1810.816	8.61125E+03	-1.00000E+00	0.00000E+00
#SumE=	3.48479E-02		

+++++

You can check, SumE is the sum of the triple differential cross sections of the 4-th column.

+++++

+++++

Now follows the triple differential cross sections for polarization experiment.

2*M0 means twice the z component of projectile, 2*(m1,m2) are those of ejectiles, particle 1 and particle 2.

+++++

#2*M0=-4 2*(m1,m2) tri_Xsec

#P1(MeV/c) (0, 0)

8097.493 4.47308E-05

8103.514 4.65350E-05

+++++

Many lines are skipped.

+++++

Some explanations

We can count the degree of freedom of the final state to be 9, for there are three particles are moving independently. Energy and momentum of the total system, 4 parameters, are defined by E_i and \mathbf{p}_i by the incident channel parameters. Five degree of freedom, 9-4, remain and they are usually chosen as detection orientation, (Ω_1 and Ω_2) and kinetic energy of particle 1, E_1 . Triple differential cross section is given as (PTP IV 2.8),

$$\frac{d^3 \sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{2\pi}{\hbar} \frac{\mu_R}{P_0} |T_{fi}|^2 \rho(E_1) \quad (6)$$

where, μ_R/P_0 is the relative velocity in the incident channel, $\rho(E_1)$ is the state density of the final state,

$$\rho_1(E_1) dE_1 d\Omega_1 d\Omega_2 = h^{-6} \frac{m_1 m_2 m_3 p_1 p_2}{(m_2 + m_3) + \frac{m_2(\mathbf{p}_1 - \mathbf{P}) \cdot \mathbf{p}_2}{p_2^2}} dE_1 d\Omega_1 d\Omega_2, \quad (7)$$

and T_{fi} is the transition matrix

$$\begin{aligned} T_{fi} = & i \sum \frac{(2\pi)^3 \hbar^2}{\sqrt{2} K_0 K k \mu_R} e^{i(\sigma_l + \delta_l + \sigma_{L_0} + \sigma_L)} \sqrt{2L_0 + 1} \langle I_0 M_0, L_0 0 | J M_0 \rangle \\ & \times \langle I M_I, L M_L | J M_0 \rangle \{ \langle s_1 m_1, s_2 m_2 | s m_s \rangle \langle l m_l, s m_s | I M_I \rangle \} \\ & \times Y_{l m_l}(\hat{\mathbf{k}}) Y_{L M_L}(\hat{\mathbf{K}}) S_{L L_0}^{J \pi}. \end{aligned} \quad (8)$$

Expression of T_{fi} is a little different form (PTP IV 2.10), where $\sqrt{\mu_\rho}$ is replaced by $\sqrt{\mu_R}$. Geometric factors in this T_{fi} is that of L-S coupling. When j-j coupling is used in 1-2 system, product of Clebsch-Gordan coefficients in the curly brackets in (8) is replaced by the following expression,

$$\langle l m_l s_1 m_1 | j m_j \rangle \langle j m_j s_2 m_2 | I M_I \rangle \quad (9)$$

$$= \sum_s \hat{j} \hat{s} \langle s_1 m_1 s_2 m_2 | s m_s \rangle \langle l m_l s m_s | I M_I \rangle W(l s_1 I s_2; j s). \quad (10)$$

This means L-S T_{fi} matrix should be summed over s with additional geometric factor of $\hat{j} \hat{s} W(l s_1 I s_2; j s)$.

Program hctak calculates S matrix at discretized wave numbers, interpolation is used to estimate arbitrary value of k and K . In this interpolation process, zero S matrix value is assumed for the outside range of k_{min} and k_{max} .

It seems that the resulting triple differential cross section is not very smooth, and some difficulty is experienced in calculating double differential cross sections.

opm

Elastic scattering cross section under central optical potential is calculated by opm.f. It is written in FORTRAN and the executable file can be made by follows,

```
|prompt> frt -o opm opm.f
```

It uses 'opm.in' and 'opm.out' for standard I/O files with logical unit numbers 5 and 6, respectively. It uses 'umtab' file for nuclear database.

input

Input data is line oriented with maximum of 80 columns. Input of **0-th** and **1st group** are formatted and the rest are format free.

0-th group TITLE with format (A50)

Like the corresponding input of hctak this line is used for column indicator.

1st group (KNTL(i), i=1, 10), TITLE with format (10I2,5X,A50).

KNTL(1) how reaction information is read.

=0: get masses etc. from TITLE of this line

=9: input follow later

KNTL(2) NPOT

specifies the number of lines to define optical potential.

KNTL(3) NPOW

specifies maximum integration radius (RMX).

< 0 input later

=0: replaced by 6

> 10 replaced by 10

= n , ($0 < n \leq 10$): RMX is defined internally as the radius where potential depth drops below 10^{-n} of the surface value.

KNTL(4) NSTEP

specify mesh size of integration (DR) to be $1/2^{NSTEP}$ of wave number at infinity.
3 or 4 seems appropriate.

This line is effective only when non-negative NSTEP is given.

KNTL(5) not used

KNTL(6) > 0 to print potential.

KNTL(7) > 0 to print radial wave functions. The output radial wave function is not reasonably normalized. You should multiply by C0, which is defined at line 603 in the source program. C0 is named as the normalization in the program.

KNTL(8) > 0 to print C-coefficients.

KNTL(9) > 0 to print $\langle V \rangle$, which is explained later.

KNTL(10) not used.

TITLE same as TITLE of the **1st group** of hctak input.

2-1 group IZ(I),IA(I),IS(I),JP(I),EM(I),I=1,2)

2-2 group IZ(3),IA(3),IS(3),JP(3),EM(3),ELAB

IZ(I), IA(I) atomic and mass numbers of projectile and target, respectively

IS(I), JP(I) twice the spin and parity of projectile and target, respectively

EM(I) masses in u, the atomic mass unit.

ELAB kinetic energy of the projectile in MeV.

2-1 and 2-2 group should be input only if KNTL(1)=1. IZ(3) to JP(3) are not used in the program, but should be input.

3rd group ISI, ISD, V, R, A

This group consists of NPOT(=KNTL(2)) lines. Optical potential is defined by using NPOT lines.

ISI =1 if this line is for the imaginary part.

ISD =1 if this line is for the surface type potential.

V, R, A specify depth, radius and diffuseness of the potential in unit of MeV or fm, respectively.

Potential type is the same as that of hctak, i.e.,

volume type is $V/(1+e)$ and surface type is $4Ve/(1+e)^2$, so V should be negative for attractive or absorptive potentials. $e \equiv \exp((r-R)/a)$. Notice that the R is not scaled by $A^{1/3}$.

4-th group DR, RMX

This line should be given if KNTL(3) is negative. DR and RMX define mesh size and maximum radius of integration in fm.

5-th group RC, LMIN, LMAX, LDEL

RC is the Coulomb charge radius. LMIN, LMAX, LDEL define the minimum, maximum and increment of orbital angular momentum of the relative motion. If zeros are given to LMIN, LMAX, LDEL, default values are used. Coulomb potential is due to the uniformly charged sphere.

6-th group ANG0, ANG1, DANG

First angle, last angle and angle increment in degree. Differential cross sections, in center of mass system, are calculated for these angles.

Sample input and output

No further explanation may be necessary for the following sample input. Those who has no experience to use this program are advised to adopt default values.

```
1 2 3 4 5 6 7 8 9 0
0 2 0 0 0 0 0 1 0 0      12C(23Al,23Al), E=1840 MeV. set F
0 0 -120 3.644 0.84 /real WS V R a
1 0 -34.02 4.928 0.69 /Imag WS V R a
6.673 0 0 0 /Rcoul Lmin, Lmax, Ldel
0.1 20 .1 /1st and last angles, angle increment [deg]
```

Output of this sample input looks like as follow. Lines sandwiched by leading '+++++' lines are comment lines added later for explanation.

```
2 4 6 8 10 title
0 2 0 0 0 0 0 1 0 0 12C(23Al,23Al), E=1840 MeV. set F
```

NUCSPE: J and pi of Z= 13 A= 23 assumed to be 0+

NUCSPE: J and pi of Z= 13 A= 23 assumed to be 0+

sys	Ename	Z	A	J pi	M(u)
1	C	6	12	0 +	11.9967
2	AL	13	23	0/2 +	23.0001
3	AL	13	23	0/2 +	23.0001

```
Elab(1+2)=1840.0000 Ecm= 630.7411 [MeV]
Eta = 1.3730 k= 15.4208 [/fm]
```

```
(Npow Nstep)=( 6 3) NRMX= 2038
```

```
DR= 8.106E-03 RMX= 1.652E+01 [fm]
```



```

(Lmin Lmax Ldel)=( 0 0 1)
new Lmax          253

Potential parameters
ISI   type   depth[MeV]   radius[fm]   dif.[fm]
0      0    -120.0000      3.6440      0.8400
1      0     -34.0200      4.9280      0.6900
      RC              6.6730

(Ang0 Ang1 Dang)=( 0.10 20.00 0.10)[deg]
+++++
Above lines may be understood without explanation.
Partial wave scattering amplitude for each L, the orbital angular momentum of
the relative motion, follow. This left(right) real number is a real(imaginary)
part of the $C_l$ given later.
+++++
# L   Part. wave scatt. amp.
#L and C2= 0   5.98531E-04   5.09855E-01
#L and C2= 1   9.18781E-03   4.96371E-01
+++++
output for L=2 to 252 are deleted
+++++
#L and C2= 252   3.32565E-07   2.28205E-08
#L and C2= 253   2.25857E-07   1.54521E-08

+++++
Differential cross section follows.
Column under 'ANG(deg)' for scattering angle in degree, 'Xsec(mb/sr)'
differential cross section in mb/sr, 'Ruth(mb/sr)' for Rutherford scattering
and the last line for the ratio of both cross sections.
+++++
#Ang(deg) Xsec(mb/sr) Ruth(mb/sr) Xsec/Ruth
0.100    3.39344E+10   3.41729E+10   9.93023E-01
0.200    2.17291E+09   2.13581E+09   1.01737E+00
+++++ line for 0.3 to 19.8 degree are deleted +++
19.900   9.66689E-04    2.22336E+01   4.34788E-05
20.000   8.56758E-04    2.17966E+01   3.93069E-05
# Xtot= 1.23874E+03[mb]

```

+++++

The last line tells the total reaction cross section in mb.

++++

Some explanation

Following Schrödinger equation for the central optical potential, V , is solved,

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V\right)\psi = E\psi. \quad (11)$$

The solution with definite angular momentum ψ_{lm} is written as follows

$$\psi_{lm}(\mathbf{r}) = \frac{1}{r} u_l(r) Y_{lm}(\hat{\mathbf{r}}). \quad (12)$$

Radial part $u_l(r)$ satisfies the following equation

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right)u_l(r) + V(r)u_l(r) = E u_l(r), \quad (13)$$

with the boundary condition of

$$u_l(0) = 0, \quad u_l(r) \rightarrow F_l + C_l\{G_l + i F_l\} \quad r \rightarrow \infty. \quad (14)$$

F_l and G_l are Coulomb wave functions. ψ is expanded by using ψ_{lm} by requesting that the incoming part of the ψ is the same as the incoming part of the Coulomb scattering. So the scattering amplitude is the sum of Coulomb scattering amplitude f_C and the one due to optical potential, which is proportional to C_l .

$$f(\theta) = f_C(\theta) + \sum_l (2l+1) e^{2i\sigma_l} C_l P_l(\cos\theta)/k \quad (15)$$

$$f_C(\theta) = -\frac{\eta}{2k \sin^2 \theta/2} e^{-i(\eta \ln \sin^2 \theta/2 + 2\sigma_0)} \quad (16)$$

Total reaction cross section σ_R is a difference of incoming and outgoing flux and are written as,

$$\sigma_R = \frac{\pi}{k^2} \sum_l (2l+1) (1 - |1 + 2i C_l|^2) \quad (17)$$

If we write ψ as follow,

$$r \chi^{(+)}(\mathbf{r}) = \frac{1}{k} \sum_l \sqrt{4\pi(2l+1)} i^l e^{i\sigma_l} u_l(r) Y_{l0}(\hat{\mathbf{r}}). \quad (18)$$

After some manipulation, we can write the following relation

$$\langle r \chi^{(+)} | V(r) | r \chi^{(+)} \rangle_{\mathbf{r}} = \frac{4\pi}{k^2} \sum_l (2l+1) |u_l(r)|^2 V(r) \quad (19)$$

This expression tells how the potential is felt by the wave function. So may be named as sensitivity function. If we integrate over radial directions, imaginary part of (19) is proportional to the total reaction cross section and $r_a \equiv \langle r \chi | r V | r \chi \rangle / \langle r \chi | V | r \chi \rangle$ gives the absorption radius.

wsf

Program wsf.f is written in FORTRAN and is designed to calculate bound and scattering state wave functions under given potential. Potential is consist of fixed and floating part. Depth of floating potential is adjusted to reproduce given binding energy. Fourier transform of the bound state wave function can be calculated. Energy dependence of the phase shift and resonance state may be calculated under the given potential.

executable program

By issuing following command to the command interpreter, you can make an executable file of wsf.f,

```
|prompt> frt -o wsf wsf.f
```

You can ‘improve’ the program by issuing ‘improve/optimize’ option to the FORTRAN compiler.

The program uses ‘wsf.in’ and ‘wsf.out’ as standard I/O files with logical unit numbers of 5 and 6. It uses ‘umtab’ with logical unit number 8 as nuclear database.

Input

One control line, which define KTWSF(1,···,5), is added just in front of the hctak input. This line is format free and has the following meaning. Rest of the input to wsf is the same as hctak.

KTWSF(1) =1 to reset all the intrinsic spins, i.e., IS(1)=IS(2)=IS(3)=0
 KTWSF(2) > 0 do not print bound state wave function
 KTWSF(3) > 0 Fourier transform of the bound state wave function
 KTWSF(4) =1 to print wave number dependence of phase shift
 KTWSF(5) Not used

functions

- 0 Calculate potential form.
- 1 Calculate bound state wave function.
- 2 Calculate Fourier transform of the bound state wave function.
- 3 Calculate scattering states and see if the sign change of $\cos \delta$ may take place, i.e., presence of resonance.
- 4 Calculate resonance energy and width if resonance is found.

Sample input and output

Following is a sample input. Lines sandwiched by the lines with leading '+++++' are comment lines.

```

0 1 0 0 0          KTWSF added
  2   4   6   8  10      | title begins
1 2 0 0 0 0 0 0 2 0      (p+22Mg)+12C, E=100.37 MeV
  system 1-2
2  5  5  1  1 /LSTAB, ISTAB, JSTAB, NBND, IDVS: Gnd, d5/2 state
0  0  0.126      /NODS, ISBE, BES: depth adjust
1  0.1348  0.1444      /NKSBIN FKSMIN FKSMAX

```

+++++

rest of the lines are deleted

Output to this input is as follow

+++++

WSF ver. 2008/09/29 by Y. Aoki

```

  2   4   6   8  10          title
1 2 0 0 0 0 0 0 2 0      (p+22Mg)+12C, E=100.37 MeV
0 1 0 0 0
  sys  Ename   Z    A    J    pi    M(u)
  1     H     1    1   1/2   +    1.0073
  2    MG    12   22    0    +    21.9930
  3     C     6   12    0    +    11.9967
          Elab((1+2)-3)=  100.3700 MeV

```

*****system 1-2 in jj coupling*****

CH	ls	2*s1	2*j1	2*s2	2*I12	Nbnd	Nkbin	k(min)	k(max)	Pid
1	2	1	5	0	5	1	1	0.1348	0.1444	1
2	0	1	1	0	1	0	1	0.1000	1.9000	1

bound states

Ch	Node	BE	isBE?
1	0	0.1260	0

System 1-2: potential parameters

Pid	I1	I2	V(MeV)	R(fm)	a(fm)	ROC(fm)
1	1	3	-7.50000	3.50255	0.65000	0.00000
1	1	1	-46.80000	3.50255	0.65000	3.50255

I1=1(2) fixed (floating) part I2=1(2) volume (surface) type

N12= 3 NR12= 300 DR12= 0.1000 fm. Lambda= 0 to 2

System 1-2 ch. ID= 1

potential parameters

I1	I2	V(MeV)	R(fm)	a(fm)	NRMX
1	3	-7.50000	3.50255	0.65000	259
2	1	-46.80000	3.50255	0.65000	259

R Coul= 3.50255

WSBND: ISBE= 0

Loop	LS	NS	NN	Vfac	BE(MeV)	FI
0	2	0	0	1.00000	0.12600	1.40247E-03
1	2	0	0	1.00140	0.12600	-5.39587E-06

<r>= 3.6883E+00 sqrt(<r*r>)= 3.9206E+00 fm

+++++

Above output lines are the same as that of hctak

Now follows the output from resonance search

It failed to locate for d5/2 spin channel

Notice the potential depth is a little modified to reproduce the input binding energy

+++++

WSRES: for Ls= 2 Btop= 5.3792 MeV k range=[0.030, 0.498]

No resonance found

+++++

proceed to locate resonance for s1/2 spin channel

+++++

System 1-2 ch. ID= 2

potential parameters

I1	I2	V(MeV)	R(fm)	a(fm)	NRMX
1	3	-7.50000	3.50255	0.65000	259
1	1	-46.86564	3.50255	0.65000	259

R Coul= 3.50255

WSRES: for Ls= 0 Btop= 2.2539 MeV k range=[0.030, 0.322]

Eres= 0.39996MeV k= 1.3572415E-01 /fm

k_c= 1.3572415E-01 +/- 6.198E-06 [/fm] : {cos(delta)=1/sqrt(2)}

del(k_c): 6.204E-06 -6.193E-06 [/fm]

+++++

one resonance is located at around 0.4 MeV with $k_{\text{res}}=0.135\ldots$ /fm.
 wave numbers for $k_{\text{res}}+ 6.204\text{E-}6$ or $k_{\text{res}}-6.193\text{E-}6$ /fm, phase
 shift changes its value by $\pi/4$ radian.

Output of this type follows until all the spin state channels are
 studied

+++++

Definitions

Fourier transform of the bound state wave function.

We write bound state wave function as follows,

$$R_{lm}(\mathbf{r}) = \frac{u_l(r)}{r} Y_{lm}(\hat{\mathbf{r}}). \quad (20)$$

Fourier transformation of R_{lm} is,

$$R_{lm}(\mathbf{k}) = (2\pi)^{-3/2} \int d\mathbf{r} R_{lm}(\mathbf{r}) e^{i\mathbf{r}\cdot\mathbf{k}}. \quad (21)$$

Fourier transform output from wsf program is as follows,

$$R_l(k) \equiv \sqrt{\frac{2}{\pi}} \int_0^\infty dr u_l(r) kr j_l(kr)/k. \quad (22)$$

Phase shift of the scattering state is defined as follows,

$$u_{lj}(r) \xrightarrow{r \rightarrow \infty} \cos \delta_{lj} F_l(kr) + \sin \delta_{lj} G_l(kr) \quad (23)$$

Resonance is located by looking for the wave number, where $\cos \delta_{lj} = 0$.