Preface

This write-up describes the preliminary version of the finite range DWBA code, DWUCK5. The program is still under development but it is in an advanced enough form to be used by others. The input format follows very closely that used by the zero range code DWUCK4 and the user should note the differences where they occur. These differences occur in the use of the control integers on card set 1 and the specification of variables on card sets 3 and 4. The distorted wave and form factor card sets remain the same except in the latter case where two sets are now required, one for the heavy particle bound state and a second one for the light particle bound state.

The program is in a multi-level overlay form and uses about the same core space as DWUCK4, namely $(24K)_{10}$ on a CDC 6400 under the RUN compiler. The present version of the program has a limit of 200 partial waves, 400 integration steps, and 40 expansion coefficients for each distorted wave. These capabilities take care of most cases even heavy ion cases where the present version has been tuned and tested. The full spin capabilities for the distorted waves will be very useful for all the light ion reactions where polarizations and asymmetries are needed.

The method of calculation of the full finite range is via the momentum expansion technique of Lowell Charlton (Phys. Rev. C 8 (1973) 146). This method has been found to be extremely efficient and fast for most cases that have been tested.

Since the program is a preliminary version there may be instances of incorrect calculations or logical bugs waiting to be found. I would appreciate any comments from the user concerning any difficulties in using the code. There are several parameters which control the accuracy of various operations. These have conveniently set default values although for any particular case

they may not be sufficient for your purposes. One convenient way of testing whether you have sufficient accuracy is to run a set of cases with increasing accuracy requirements and see how much the cross section changes in your region of interest. Of course increased accuracy requires a penalty of increased running time. Another way to test is to run a zero range case for a projectile ℓ transfer of zero and compare the results with DWUCK4.

I wish to thank Professor Rost and Dr. Charlton for their help and useful suggestions during the development of this code.

Good luck!!

Sincerely,

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Card Set 1 (1 card)

ICON(16), ALPHA
FORMAT (16I1, 4X, 15A4)

i	ICON(i)	Function
1	0	Do not read in card set 2 (angle data)
	1,2	Read in card set 2
	9	Calls EXIT to terminate program
2		Not used at present
3	0	Use different form factor for each L transfer. (Read in one set of card set 7 and card set 8 for each L transfer.)
	1	Same as ICON(3)=0 except the cross section is the coherent sum of amplitudes from each L transfer
4	0	Prints form factor before finite range and non-local corrections
	1	Suppresses form factor printing
5	0	Prints elastic S matrix = $(\exp(2i\delta_{\ell j})-1)/2i$
	≠0	Suppresses elastic S matrix print-out
6	0	Suppresses elastic scattering cross section print-out
	1	Prints elastic scattering cross sections
	N>1	Prints and plots elastic scattering cross sections. Plot is an N-decade log scale.
7	0	Suppresses radial matrix element print-out
	≠0	Prints radial matrix elements
8	0	Suppresses inelastic scattering amplitude print-out
	≠0	Prints inelastic scattering amplitudes
9	0	No plot of inelastic cross section
	N	Plots inelastic cross section with N-decade log scale
A(10)	0	Usual non-relativistic kinematics
	≠0	Relativistic kinematics
B(11)	0	Reads in a full set of form factor cards for 2nd bound state and computes $\phi_\ell(r)$.
	1	Zero range option. Sets $F_\ell(q)/q^\ell$ = -100.0 for 2nd bound state.
	2	External Form factor in momentum representation
C(12)	0	Suppresses radial wave function of DW print-out
	1	Prints out expansion coefficients for radial wave function of DW
D(13)	0	Uses full range of angles in Fourier transform Δq
	1	Cutoff at 90° used in Fourier transform Δq

E(14)	0	Program does entire calculation for case
	1	Program discontinues case after distorted wave expansion
F(15)	0	Suppresses print-out or K(r)**2 of distorted waves
	≠0	Prints out K(r)**2 of distorted waves
G(16)	0	Not used at present

Alpha — Any 60 alpha numeric characters to identify the run, beginning in column 21 of the card

Card Set 2 (1 card)

Angle input

If ICON(1)=1 the input of card set 2 is interpreted as

No. of angles, First angle, Angle increment.
FORMAT (3F8.4)

If ICON(1)=2 the input of card set 2 is interpreted as

Last angle, First angle, Angle increment.
FORMAT (3F8.4)

The program has a set of standard angle data pre-stored for the interval 0^{o} to 180^{o} in 5 degree intervals which will be used until changed by reading in a card set 2. The first angle may be +00.00 since the program will check for a zero angle when computing the elastic scattering cross sections.

Card Set 3

LMAX, NLTR

FORMAT (2I3)

LMAX the maximum partial wave used in the cross section. The limit is given by 200.

NLTR the number of angular momentum transfers allowed per case. A maximum of 8 is allowed.

Card Set 4

DR, RMAX, (ACC(I),I=1,6) FORMAT (8F8.4)

DR integration step size
±RMAX upper cutoff on the radial wave functions

(Card Set 4 continued on next page)

Card Set 5 (minimum of 2 cards) — Initial distorted wave data set

Card 1 (Kinematic card)

E, MP, ZP, MT, ZT, R_{oc}, AC, PNLOC, 2*FS, QCODE
FORMAT (10F8.4)

E	Laboratory energy of initial projectile (must be non-zero
MP	Projectile mass (in AMU units)
ZP	Projectile charge
MT	Target mass (in AMU units)
ZT	Target charge
R_{oc}	Coulomb charge radius ($R_c=R_{oc}\ MT^{1/3}$)
AC	Coulomb charge diffuseness (not used)
PNLOC	Non-local range parameter
2*FS	Twice the projectile intrinsic spin
QCODE	Q option (used for card set 6)

Cards (2-N) (Potential cards)

OPT, VR, R_{OR}, AR, VSOR, VI, R_{OI}, AI, VSOI
FORMAT (10F8.4)

OPT	Potential option
VR	Real well depth
R_{OR}	Real well radius ($R_R=R_{OR}\ MT^{1/3}$)
AR	Real well diffuseness
VSOR	Real well Thomas spin orbit factor
VI	Imaginary well depth
R_{OI}	Imaginary well radius ($R_I=R_{OI}\ MT^{1/3}$)
AI	Imaginary well diffuseness
VSOI	Imaginary Thomas spin orbit factor
POWR	Extra variable used for some potential options (described later in potential option descriptions)

Any number of potential cards may be used and the resulting potential will be the sum of potentials defined on the cards. If OPT is a negative option that option will be computed and the potential string will be ended and the next card set will be read in. If OPT is zero, no potential will be computed and the next card set will be read in.

Card Set 4 continued

The limitation on DR and RMAX is RMAX/DR ≤ 400. A plus sign for RMAX allows the program to override RMAX by built-in criteria up to the maximum of 400 integration points allowed by storage. The minus sign defeats the override provision and uses |RMAX| as the upper cutoff on the integration of the distorted waves and radial integrals.

ACC(1) Controls wave number spread for initial distorted wave. Default value = 1.0.

ACC(2) Controls wave number spread for final distorted wave. Default value = 1.0.

ACC(3) Controls variable wave number width for initial distorted wave. Default value = 0.0.

ACC(4) Controls variable wave number width for final distorted wave. Default value = 0.0.

ACC(5) Controls value of classical turning point search for initial distorted wave. Default value = 1.0.

ACC(6) Controls value of classical turning point search for final distorted wave. Default value = 1.0.

Card Set 6
(minimum of
2 cards)

Final distorted wave data set

Card 1 is the same as in card set 6 except the parameter E is interpreted in three different manners depending upon the QCODE parameter.

QCODE > 0.0	E is ELAB of time reversed reaction
QCODE = 0.0	E is Q of reaction
QCODE < 0.0	E is the partial Q where Q = E + QCODE

This last option allows one to enter the ground state Q in the field for E and allows minus the excitation energy of the state to be entered in the field of QCODE so that the total Q is computed by the program.

The remaining cards of set 6 are defined in the same manner as cards (2-N) for card set 5.

Card Set 7 (minimum of 3 cards)

Form factor for first bound state.

Card 1 (kinematic card)

E, MP, ZP, MT, ZT, R_{oc}, AC, PNLOC, 2*FS
FORMAT (10F8.4)

E	Binding energy of single particle
MP	Mass of single particle
ZP	Charge of single particle
MT	Mass of core binding single particle
ZT	Charge of core binding single particle
R_{oc}	Coulomb charge radius ($R_c=R_{oc}MT^{1/3}$)
AC	Coulomb charge diffuseness (not used)
PNLOC	Non-local range parameter
2*FS	Not used

Card(2-N) (Potential cards)

Same as for card sets 5 and 6 of the distorted waves.

If E ≠ 0.0, the form factor computes a single particle orbital bound by E in the potential defined by the potential cards. In this case an additional card is needed to define the angular momentum quantum numbers of the orbital.

Card (N+1) (quantum number card)

FN, FL, 2*FJ, 2*FS, VTRIAL, FISW, DAMP
FORMAT (10F8.4)

FN	Number of nodes excluding the origin and infinity
FL	Orbital angular momentum of the particle
2*FJ	Twice the total angular momentum of the particle
2*FS	Twice the intrinsic spin
VTRIAL	Scaling factor for the bound state potentials
FISW	Search control for bound state
DAMP	Damping factor for single particle wave function

FISW = 0 Search on well depth, i.e. VTRIAL, for fixed binding energy
1 Search on binding energy, i.e. E, for fixed potentials
2 No search (for E > 0 only)

DAMP≠00 A damping factor exp(-DAMP*r) multiplies the "bound" state function and the function is then renormalized to 1.0.

The total potential is the product of VTRIAL and the real part of the potential defined by cards (2-N). For the usual bound state VTRIAL*VR must be less than zero. If VTRIAL is left blank a standard value of VTRIAL = +60.0 is used. In this case VR should be -1.0.

If E=0.0, a form factor defined by the potential options is computed and card N+1 should be omitted.

Card Set 8
(minimum of 3 cards)

Form factor for second bound state. This bound state gives the interaction potential for the transfer reaction.

ICON(11) = 0 Bound state calculation
These cards are identical to card set 7.

ICON(11) = 1 Zero range option
Only card (N + 1), the quantum number card, is specified.

ICON(11) = 2 External Fourier transform read-in option

Card 1

FN, FL, 2*FJ, 2*FS
FORMAT (4F8.4)

FN = number of points read in at intervals Δq=0.05 fm^{-1} and starting with first $q = \Delta q = 0.05$ fm^{-1}.

Card 2-N

($F(q_N)$, N=1, FN)
FORMAT (5E16.7)

OVERLAY	0,0	Main control overlay
DWUCK5		Main control program
VCC		Clebsh-Gordan coeff. routine
PHASEF		Computes $(-1.0)^N$
YXFCT		Computes N!/M!
RACAH		Racah coeff. routine
DELR		Triangular function routine
WINEJ		Nine-J coeff. routine
CUDATE		TIME and DATE decoder
LGNDR		Legendre polynomial routine
DWPLOT		Printer plot routine
OVERLAY	1,0	First overlay
ADWUCK		First control program
OVERLAY	1,1	Sublevel 1 overlay
AADWUCK		Read in data cards and sets up form factors
FORMF		Kinematics and form factor control
POTS		Form factor option routine
BIND		Bound state routine
COU		Coulomb function routine
OVERLAY	1,2	Sublevel 2 overlay
INTEG		Distorted wave calculation and expansion program
INVERT		Simultaneous equation solution routine
BES		Bessel function routine
OVERLAY	1,3	Sublevel 3 overlay
ELSIG		Elastic scattering program
POLFCT		Polarization routine
OVERLAY	2,0	Second overlay
BDWUCK		Second control program
EXPAND		Calculates Fourier transforms of bound states
RADINT		Calculates radial integrals for DWBA
XFORM		Calculates Legendre expansion of form factor product
LEGAUS		Gauss-Legendre integration coefficient routine
OVERLAY	3,0	Third overlay
CDWUCK		Cross section control
BETAFN		Inelastic scattering amplitude routine
INSIG		Inelastic cross section routine
POLFCT		Polarization routine

pickup $\frac{d\sigma}{d\Omega} = \mathcal{S} A \sigma_{DWS}$

stripping $\frac{d\sigma}{d\Omega} = \mathcal{S} a \frac{2J_f+1}{2J_i+1} \sigma_{DWS}$

$\mathcal{S}$: Target spectroscopic factor

a : Projectile spectroscopic factor

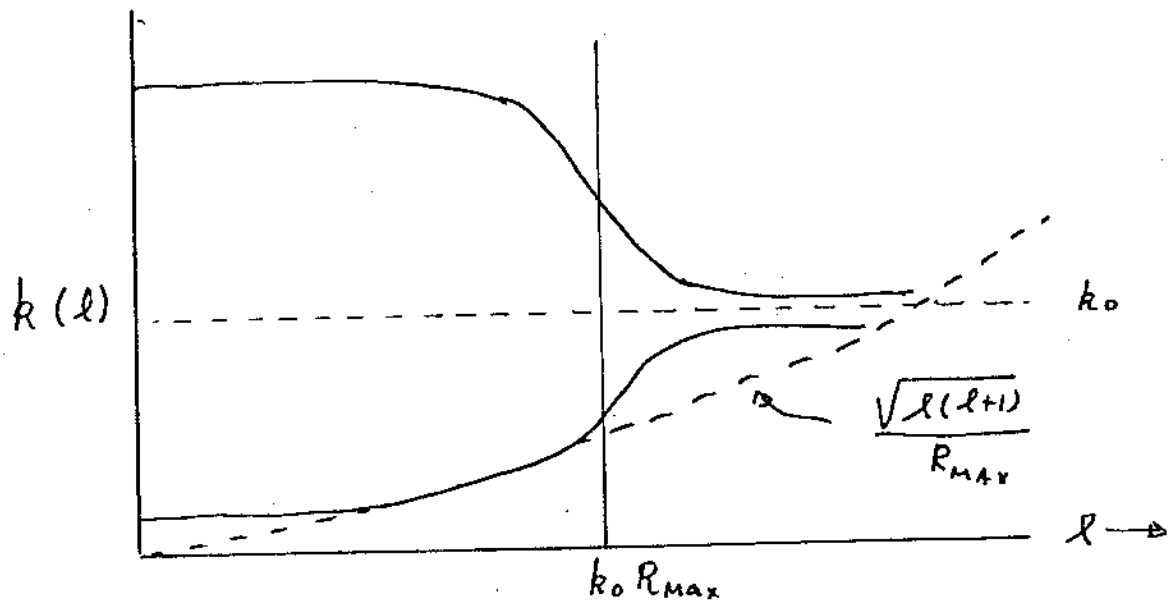
DWUCK5

General:

This is a short note to describe the function of the accuracy parameters in DWUCK5 and to aid in assigning them. I hope eventually to do all this automatically within the program with a set of default algorithms.

To begin, one must have an idea of what the momentum dispersion of each partial wave looks like. This is shown in fig. 1.

Figure 1



The low partial waves see the full potential and hence can have momentum components which differ considerably from the free value of k_o. These additions are not only from the increase in the local momentum inside the potential but also are from absorption effects of the imaginary part of the potential. Hence deep optical potential families will require more expansion coefficients than will the shallow family potentials. The high partial waves do not see the nuclear part of the potential and receive a small dispersion from the coulomb potential.

A rough estimate for the number of expansion coefficients needed where the real potential causes the dispersion is

$$n = \sqrt{\frac{2\mu}{\hbar^2}(E+V(0))} \ *RMAX/\pi \qquad V(0) > E$$

$$n = \sqrt{\frac{2\mu}{\hbar^2}(2V(0))} \ *RMAX/\pi \qquad V(0) < E$$

where RMAX is the expansion radius. From this we can see that the smallest RMAX that gives good accuracy should be used so that the number of expansion coefficients is minimized.

Accuracy:

The general accuracy required for the expansion of the distorted waves is variable although a figure less than .2-.3 percent is the value one should strive for. A badly mismatched reaction case may require that the waves be expanded to .01 or even .001 percent to give acceptable results for the cross section. A check with DWUCK4 using the zero range option ICON(11)=1 may be advised. Of course an increased accuracy beyond the needs of the problem will carry a heavy penalty in increased computing time and the time required is roughly proportional to the product of the maximum number of expansion coefficients in each distorted wave.

Accuracy Parameters:

There are three accuracy parameters for each partial wave and this section will describe their function and general rules for their use.

ACC(1) and ACC(2):

This set scales the width of the expansion range about the central momentum value k. If k_{max} is the maximum momentum found in the well from r=RMAX to $r=\ell/k_o$ then for that ℓ, $k_{upper}=SQRT(k_o^2+(k_{max}^2-k_o^2)*ACC(N)**2$. Similarly the lower limit to the expansion is extended from the minimum momentum k_{min} to $k_{lower}=SQRT(k_o^2+(k_{min}^2-k_o^2)*ACC(N)**2)$.
For some cases ACC(N) needs to be set to values of 1.2→1.5 over the default value of 1.0 in order to achieve the necessary accuracy for the low partial waves.

ACC(5) and ACC(6)

In many cases the low and high partial waves are expanded with satisfactory accuracy but the transition partial waves with $\ell \sim kR$ have a relatively large error value. Rather than increase ACC(1) and ACC(2) which gives more accuracy than is needed for the low partial waves and at the expense of increased computation time one can shift the effective expansion range of fig. 1 to the right (or left) by searching the potential not to $r=\ell/k_o$ but to $r=(\ell-ACC(N+4))/k_o$. This will not affect the very low and very high partial waves in the number of expansion terms needed but will increase the number of terms for those partial waves about the transition region. Thus one increases the accuracy for those partial waves only. It is hoped that a better expansion algorithm can be found which will eliminate the need for this parameter.

ACC(3) and ACC(4)

These are perhaps the most difficult of the parameters to understand and use. Their function is to increase the linear dependence (or non-orthogonality) between the expansion function, $j_\ell(k_n r)$, so to eliminate some boundary

condition difficulties at RMAX. This allows one to achieve a greater accuracy in the expansions with the same or fewer number of terms. These parameters set a non-constant wave number spacing by the formula

$$k_n = (\pi/RMAX)*T1*(1.0-\Gamma**2/(3.0*(\Gamma**2*T1**2)+k_o$$

where

$\Gamma = 5.0*ACC(N+2)$
$T1 = n-n_o$
n_o =number of central momentum

A value for ACC(N+2) of zero gives the usual equal spacing of wave numbers.

In general one can tolerate a degree of non-orthogonality between the expansion functions and this tolerance becomes smaller as the number of terms needed for the expansion increases. A useful check may be made. This is to inspect the quality of the orthogonalization matrix of the expansion functions which must be inverted. The value of DET is the determinant of this matrix where 1.0 denotes an orthogonal expansion set. If the value of DET becomes smaller than 10^{-4} or 10^{-5} one must look at the contributions to the norm of the expanded function. If you take the default value of zero for ICON(12) you will get a list of essentially the expansion coefficients squared, $|a_n|^2$. The error of the expansion is

$$ERR = 100*(1-0 - \Sigma_n |a_n|^2).$$

Because of the non-orthogonality some $|a_n|^2$ may be negative. If any, at least for the partial waves in the transition region and below, are less than -0.02 or so the value of ACC(N+3) must be decreased. The inversion routine INVERT will try to remove rows and columns of the matrix for the lowest wave numbers to try to circumvent this problem. This number of removals is given by AUG. However, this may not be sufficient and ACC(N+3) must be decreased.

A useful rule to approximately preset this accuracy parameter is for expansion coefficients

$n \leq 20$ ACC(N+2) = 1.0
$n > 20$ ACC(N+2) = 1.0 - (n-20)/30

These settings depend upon the particular case and are given only as a rough guide.