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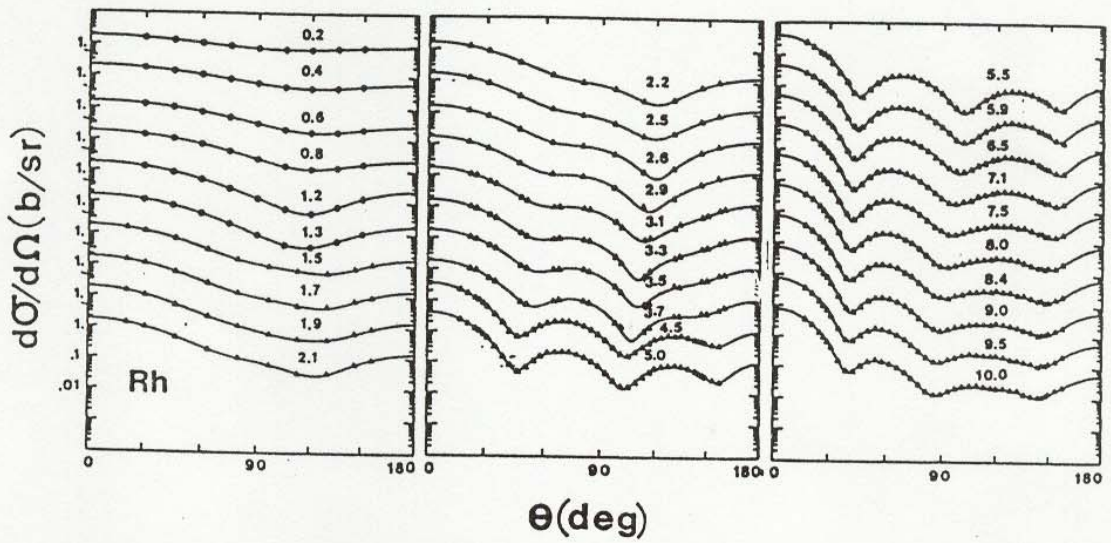
Technical note on:-

DISPERSION CONTRIBUTIONS TO NEUTRON REACTIONS

by

R. D. Lawson and A. B. Smith

April, 2001



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Technical note on:-

DISPERSION CONTRIBUTIONS TO NEUTRON REACTIONS*

by

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Simple formulation of dispersion effects in neutron reactions.

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Technical Note On:-

DISPERSION CONTRIBUTIONS TO NEUTRON REACTIONS

It is well known that there is a dispersion relationship linking the real and imaginary optical-model potentials and reflecting causality ([MNS86], [Hod94], [Sat83]). This relationship can be expressed as

$$J(E) = J_{hf}(E) + \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{J_w(E')}{E - E'} dE', \qquad (1)$$

where J(E) is the strength of the total real potential, $J_{hf}(E)$ is the strength of the local-equivalent Hartree-Fock interaction, $J_w(E)$ is the strength of the imaginary potential, and "P" denotes the principal-value integral (herein, unless otherwise stated, all potential strengths are expressed as volume-integrals per nucleon). The integral of Eq. 1 can be broken into two parts, a surface component denoted by $\Delta J_{sur}(E)$ and a volume component given by $\Delta J_{vol}(E)$, where

$$\Delta J_{sur}(E) = \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{J_{sur}(E')}{E - E'} dE' \qquad (2)$$

and

$$\Delta J_{vol}(E) = \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{J_{vol}(E')}{E - E'} dE', \qquad (3)$$

and where $J_{sur}(E')$ and $J_{vol}(E')$ are surface- and volume-imaginary potential strengths, respectively. Clearly, J(E) then becomes

$$J(E) = J_{hf}(E) + \Delta J_{vol}(E) + \Delta J_{sur}(E) \qquad (4)$$

and

$$J(E) = J_{eff}(E) + \Delta J_{sur}(E), \qquad (5)$$

where $J_{eff}(E)$ is obviously the sum of the first two terms of Eq. 4. Thus, in order to self-consistently interpret neutron-reaction data at energies $\approx < 30$ MeV one must have some way of evaluating $\Delta J_{sur}(E)$ and $\Delta J_{vol}(E)$. Complex approximations can be found in the literature, involving a number of assumptions. What is given here is an approach roughly outlined approximately a decade ago [LGS87]. It is

simple, effective, and has been used a number of times by the Argonne Group. With reasonable assumptions as to potential geometric forms, the concepts described here can be easily implemented using the spherical optical-model code ABAREX ([LS98], [Smi99]) and the coupled-channels-model code ECIS96 [Ray96]. It is a proven and useful method which is documented here to assure that it does not vanish into the mists of time.

In the following paragraphs the basic assumptions, the algebraic manipulations and the resulting formulas are set forth, and an example given. There follows a short FORTRAN program which will calculate the integrals of Eqs. 2 and 3, using reasonable formulations of the imaginary potential. The net qualitative effect of the dispersion relation on neutron-induced reactions at energies of $\approx < 30$ MeV is to add a fraction of both the surface- and volume-imaginary potentials to the real potential. The attached FORTRAN code will calculate both the total and surface fraction of these contributions as a function of energy. The ABAREX optical-model program will directly utilize the surface component in a wide range of neutron calculations using the keyword DISP" as discussed in refs. [LS98], and [Smi99]. The surface, volume and total integrals of Eqs. 1, 2 and 3 are also provided by the program and can be applied to a wide range of dispersive considerations.

The present procedure assumes the energy dependence of the imaginary potential strength illustrated in Fig. 1. It was assumed that the imaginary potential was symmetric about the Fermi Energy ($-E_f$) [JLM77], (herein the absolute value of the Fermi Energy is used). It was further assumed that from $-E_f \rightarrow 0$ the energy dependence of the surface-imaginary potential follows a parabolic behavior [JLM77], and concurrently the volume-imaginary potential is zero. From zero energy to some energy E_n the imaginary-potential strength was taken to be entirely a surface term and to increase linearly with energy as more channels open. Experimental analysis indicates that E_n is probably in the $20 \rightarrow 30$ MeV range, although some experimental interpretations extend the imaginary volume absorption to lower energies [WG86]. From E_n the surface-imaginary strength was assumed to fall linearly to zero at some energy E_v. E_v is uncertain but is reasonably in the range of $50 \rightarrow$ several-hundred MeV. Concurrently, the volume absorption rises linearly from zero at E_n to J_v at E_v. Beyond E_v the J_v was assumed to be constant to infinity. These assumptions are quite reasonable and supported by experimental evidence. However, other linear or non-linear representations can be used, if the numerical formalism is modified accordingly.

Consider the integral in Eq. 2 over the energy range x where $-2E_f \leq x \leq 0$ of Fig. 1. This range consists of sections "A" and "B" of Fig. 1. In this energy range the parabolic behavior of J_{sur} is given in Table 1. This behavior implies that the integral of Eq. 2 in regions A or B of Fig. 1 is proportional to I(E) where

$$
\begin{aligned}
I(E) &= P \int \frac{(x+E_f)^2}{(x-E)} \cdot dx \\
\text{"} &= P \int \frac{(x^2+2xE_f+E_f^2)}{(x-E)} \cdot dx \\
\text{"} &= P \int \frac{x(x-E)+(x-E)(2E_f+E)+(E+E_f)^2}{(x-E)} \cdot dx. \qquad (5)
\end{aligned}
$$

The only term in this evaluation that can lead to trouble is the logarithmic integral involving the term proportional to $(E+E_f)^2$ and this occurs when E lies in the range of the integration. In particular, consider the interval $-E_f \leq x \leq 0$. If E does not lie in this region then

$$
P \int_{-E_f}^{o} \frac{dx}{(x-E)} = \ln(x-E)\Big|_{-E_f}^{o} = \ln\left[\frac{E}{(E+E_f)}\right]. \qquad (6)
$$

On the other hand, if E does lie in the integration range then

$$
\begin{aligned}
P \int_{-E_f}^{o} \frac{dx}{(x-E)} &= \lim_{\varepsilon \to o} \left[\int_{-E_f}^{E-\varepsilon} \frac{dx}{(x-E)} + \int_{E+\varepsilon}^{o} \frac{dx}{(x-E)} \right] \\
\text{"} &= \lim_{\varepsilon \to o} \left[\ln\left(\frac{-\varepsilon}{-E_f-E}\right) + \ln\left(\frac{-E}{\varepsilon}\right) \right] \\
\text{"} &= \lim_{\varepsilon \to o} \ln\left[\left(\frac{\varepsilon}{+E_f+E}\right)\left(\frac{-E}{\varepsilon}\right)\right] \\
\text{"} &= \ln\left[\frac{-E}{E_f+E}\right]. \qquad (7)
\end{aligned}
$$

But E, by supposition, is a negative number between 0 and $-E_f$ so that the argument of the logarithm is positive and the only effect of the principal-value condition is that for any value of E, either inside or outside the range of integration, this term becomes $\ln\left|\frac{E}{E+E_F}\right|$, where $|\ldots|$ stands for the absolute value of the enclosed quantity. The value of this integral in

regions A and B of Fig. 1 is given by $\Delta J_{sur}(E)$ in Table 1.

The contributions to $\Delta J_{sur}(E)$ and $\Delta J_{vol}(E)$ in the other regions shown in Fig. 1 can be evaluated by similar methods, and the corresponding analytic expressions are given in Table 1.

In order to find the total contribution the imaginary potential makes to the real optical-model potential one must sum up the entries shown for the various regions, as given in Table 1. These include the various volume contributions, $\Delta J_{vol}(E)$. In particular, the volume contributions in the "G" and "H" regions are evaluated in the limit $c \to \infty$. Thus, "G" plus "H" are

$$\begin{aligned}
\Delta J_{vol}(E)(\text{regions G+H}) &= \frac{J_v}{\pi} \lim_{c\to\infty} \left[\ln\left|\frac{c-E}{E_v-E}\right| + \ln\left|\frac{2E_f+E_v+E}{c+E}\right| \right] \\
\text{"} \qquad &= \frac{J_v}{\pi} \lim_{c\to\infty} \left[\ln\left|\frac{c-E}{E_v-E}\right| \cdot \left|\frac{2E_f+E_v+E}{c+E}\right| \right] \\
\text{"} \qquad &= \frac{J_v}{\pi} \ln\left|\frac{2E_F+E_v+E}{E_v-E}\right| . \qquad (8)
\end{aligned}$$

Therefore, $\Delta J_{vol}(E)$, Eq. 3, becomes

$$\Delta J_{vol}(E) = \frac{J_v}{\pi(E_n-E_v)} \left[(E_n-E) \ln\left|\frac{E_v-E}{E_n-E}\right| + (2E_f+E_n+E) \ln\left|\frac{2E_f+E_n+E}{2E_f+E_v+E}\right| \right.$$
$$+ \left. (E_n-E_v) \ln \left|\frac{2E_f+E_v+E}{E_v-E}\right| \right. \qquad (9)$$

In practice, since J_{hf} in Eq. 1 is not well known, one has the option of assuming the real optical-model potential emerging from a fit to neutron reaction data is already the sum of $J_{hf}(E)$ and $\Delta J_{vol}(E)$. On the other hand, since the radius and diffuseness of the volume absorption may be different than those of the real potential, if one wants to be self consistent one should iterate on the problem.

One can calculate the total real surface potential, $\Delta J_{sur}(E)$ of Eq. 2, by summing the contributions to $\Delta J_{sur}(E)$ given in Sections A through F of Table 1. When the keyword "DISP", and associated ratio numerical values calculated by the program of the Appendix, is included in the input of the spherical optical-statistical model code ABAREX ([LS98],[Smi99]) the

contribution of $\Delta J_{sur}(E)$, discussed above, will automatically be calculated. ΔJ_{sur} and ΔJ_{vol} can also be employed in applications by using well known equations [Elt58] to convert strengths in volume-integrals-per-nucleon to potential magnitudes, assuming geometric shapes of the potentials (e.g. Saxon-Wood real form and Saxon-Wood-derivative imaginary form). The same results can be obtained with ABAREX and some other codes (e.g. ECIS96 [Ray96]) if the input parameters are suitably arranged.

It has been repeatedly shown that surface dispersive effects in neutron-induced reactions at lower energies (e.g., $\approx <$ 30 MeV) have a substantive impact on the processes and should be included in the calculations. There is also a volume contribution due to dispersive effects as set forth in Eq. 3 and Table 1. It can be calculated as illustrated in the example given below. However, as pointed out above, it can not be experimentally separated from the energy dependence of the local-equivalent Hartree-Fock potential or from the possible energy dependence of the nucleon-nucleon force.

The appendix to this Note is a small FORTRAN program which will evaluate the above equations and derive the "DISP" ratio for ABAREX or other model calculations. Certainly, other methods of evaluating the equations of Table 1 are possible. In following such alternate courses attention must be given to the poles of the various equations of Table 1. The results obtained with the program of the appendix are illustrated in Figs. 2 and 3 using a representative experimentally-derived potential for ^{121}Sb as described in ref. [Smi00]. The illustrative calculations assumed a Saxon-Woods-derivative surface-imaginary potential strength given by

$$J_w(E) = 45.63 + 1.797 \cdot E \quad (\text{MeV-fm}^3) \qquad (10)$$

to an E_n of 25 MeV. Above 25 MeV it was assumed that the surface component of the imaginary potential linearly fell to zero at 60 MeV. Concurrently, the volume absorption strength linearly increased from zero at 25 MeV to 75 MeV-fm^3 at 60 MeV and then remained constant to higher energies. This behavior is the same as that schematically illustrated in Fig. 1. The Fermi Energy was taken to be $|7.86|$ MeV. The ΔJ_{sur} of Eq. 2 and the ΔJ_{vol} of Eq. 3 are indicated in Fig. 2. ΔJ_{vol} of Fig. 2 illustrates its approximately linear energy dependence, as cited above. Using ΔJ_{tot} of Fig. 2, one can obtain the fraction of the total imaginary strength that is added to the real potential due to dispersion effects, as illustrated by the ΔJ_{tot} curve of Fig. 3. This contribution will include both a

Table 1. Parameterizations of dispersion contributions in the eight energy regions of Fig. 1.

Integral, Region A

$$J_{sur}(x) = \frac{J_o}{E_f^2}(x + E_f)^2$$

$$\Delta J_{sur}(E) = \frac{J_o}{E_f^2}\frac{1}{\pi}\left[-\frac{E_f^2}{2} + E_f(2E_f+E) + (E+E_f)^2 \ln|E/(E_f+E)|\right]$$

$$J_{vol}(x) = 0$$

$$\Delta J_{vol}(E) = 0$$

Integral, Region B

$$J_{sur}(E) = \frac{J_o}{E_f^2}(x+E_f)^2$$

$$\Delta J_{sur}(E) = \frac{J_o}{E_f^2}\frac{1}{\pi}\left[\frac{E_f^2}{2} + E_f E + (E+E_f)^2 \ln|(E_f+E)/(2E_f+E)|\right]$$

$$J_{vol}(x) = 0$$

$$\Delta J_{vol}(E) = 0$$

Integral, Region C

$$J_{sur}(x) = \frac{1}{E_n}\left[J_o E_n + (J_n - J_o)x\right]$$

$$\Delta J_{sur}(E) = \frac{1}{\pi}\left[(J_n - J_o) + \left(J_o + \frac{(J_n - J_o)E}{E_n}\right)\ln\left|\frac{E-E_n}{E}\right|\right]$$

$$J_{vol}(x) = 0$$

$$\Delta J_{vol}(E) = 0$$

Integral, Region D

$$J_{sur}(x) = \frac{1}{E_n}\left[J_o E_n + (J_o - J_n)(x+2E_f)\right]$$

$$\Delta J_{sur}(E) = \frac{1}{E_n}\frac{1}{\pi}\left[(J_o - J_n)E_n + \left[J_o E_n + (2E_f+E)(J_o - J_n)\right]\ln\left|\frac{2E_f+E}{2E_f+E+E_n}\right|\right]$$

$$J_{vol}(x) = 0$$

$$\Delta J_{vol}(E) = 0$$

Integral, Region E

$$J_{sur}(x) = \frac{J_n}{E_n-E_v}(-E_v+x)$$

$$\Delta J_{sur}(E) = \frac{J_n}{(E_n-E_v)}\frac{1}{\pi}\left[(E_v-E_n)+(E-E_v)\ln\left|\frac{E_v-E}{E_n-E}\right|\right]$$

$$J_{vol}(x) = \frac{J_v}{E_n-E_v}(E_n-x)$$

$$\Delta J_{vol}(E) = \frac{J_v}{(E_n-E_v)}\frac{1}{\pi}\left[(E_n-E_v)+(E_n-E)\ln\left|\frac{E_v-E}{E_n-E}\right|\right]$$

Integral, Region F

$$J_{sur}(x) = \frac{J_n}{E_v-E_n}(2E_f+E_v+x)$$

$$\Delta J_{sur}(E) = \frac{J_n}{(E_v-E_n)}\frac{1}{\pi}\left[(E_v-E_n)+(2E_f+E_v+E)\ln\left|\frac{2E_f+E_n+E}{2E_f+E_v+E}\right|\right]$$

$$J_{vol}(X) = \frac{J_v}{E_n-E_v}(2E_f+E_n+x)$$

$$\Delta J_{vol}(E) = \frac{J_v}{(E_n-E_v)}\frac{1}{\pi}\left[(E_v-E_n)+(2E_f+E_n+E)\ln\left|\frac{2E_f+E_n+E}{2E_f+E_v+E}\right|\right]$$

Integral, Region G

$$J_{sur}(x) = 0$$

$$\Delta J_{sur}(E) = 0$$

$$J_{vol}(x) = J_v$$

$$\Delta J_{vol}(E) = \frac{J_v}{\pi}\lim_{c\to\infty}\left[\ln\left|\frac{c-E}{E_v-E}\right|\right]$$

Integral, Region H

$$J_{sur}(x) = 0$$

$$\Delta J_{sur}(E) = 0$$

$$J_{vol}(X) = J_v$$

$$\Delta J_{vol}(E) = \frac{J_v}{\pi}\lim_{c\to\infty}\left[\ln\left|\frac{2E_f+E_v+E}{c-E}\right|\right.$$

In the limit $c\to\infty$

$$\Delta J_{vol}(E) \text{ for regions G+H} = \frac{J_v}{\pi}\ln\left|\frac{2E_f+E_v+E}{E_v-E}\right|$$

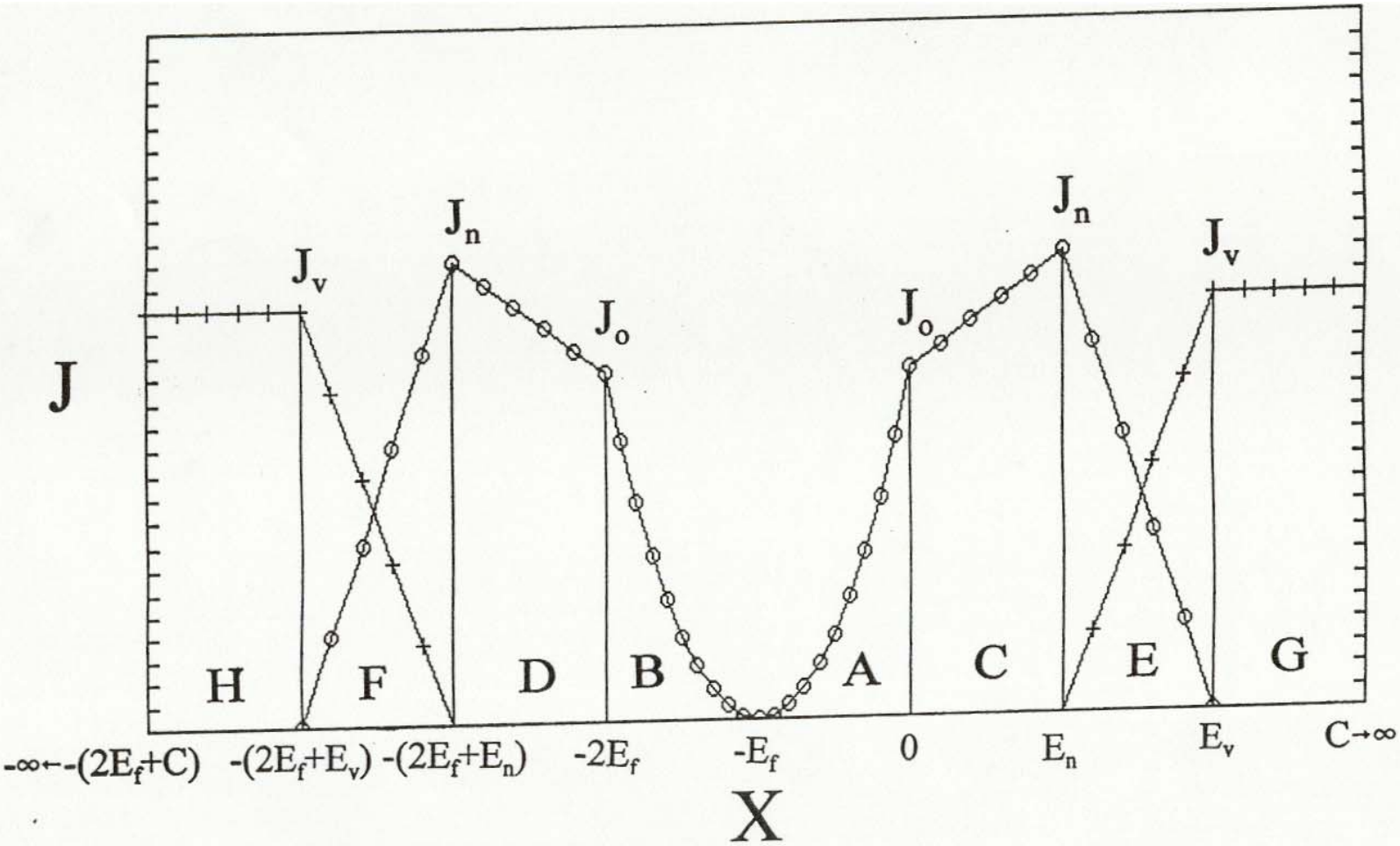

Fig. 1. Schematic diagram of the imaginary-potential energy dependence, as described in the text. "O" symbols indicate surface components of the potential, and "+" symbols the volume components.

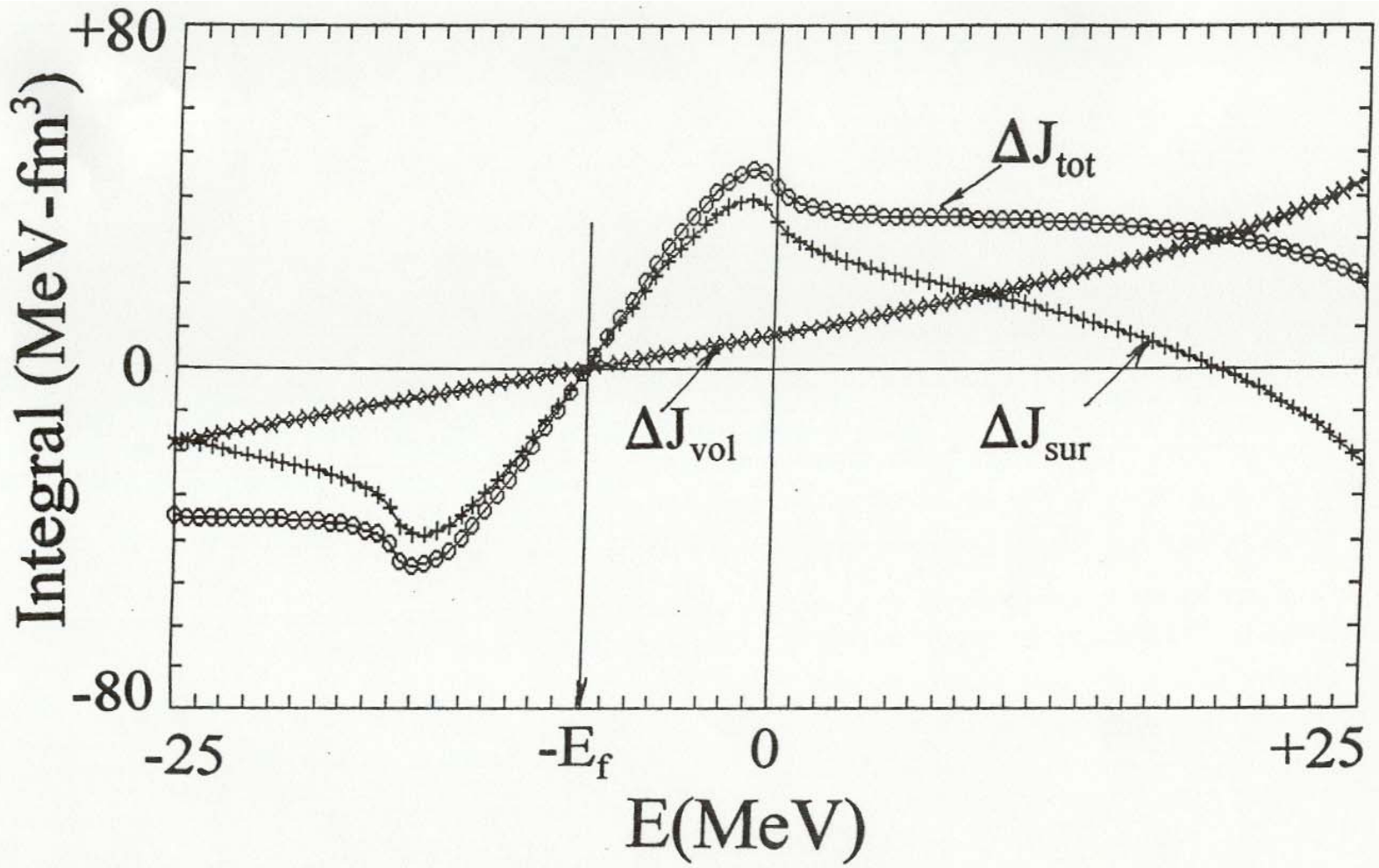

Fig. 2. Dispersive integral contributions as discussed in the text. ΔJ_{sur}, ΔJ_{vol} and ΔJ_{tot} refer to surface, volume and total dispersive contributions, as discussed in the text.

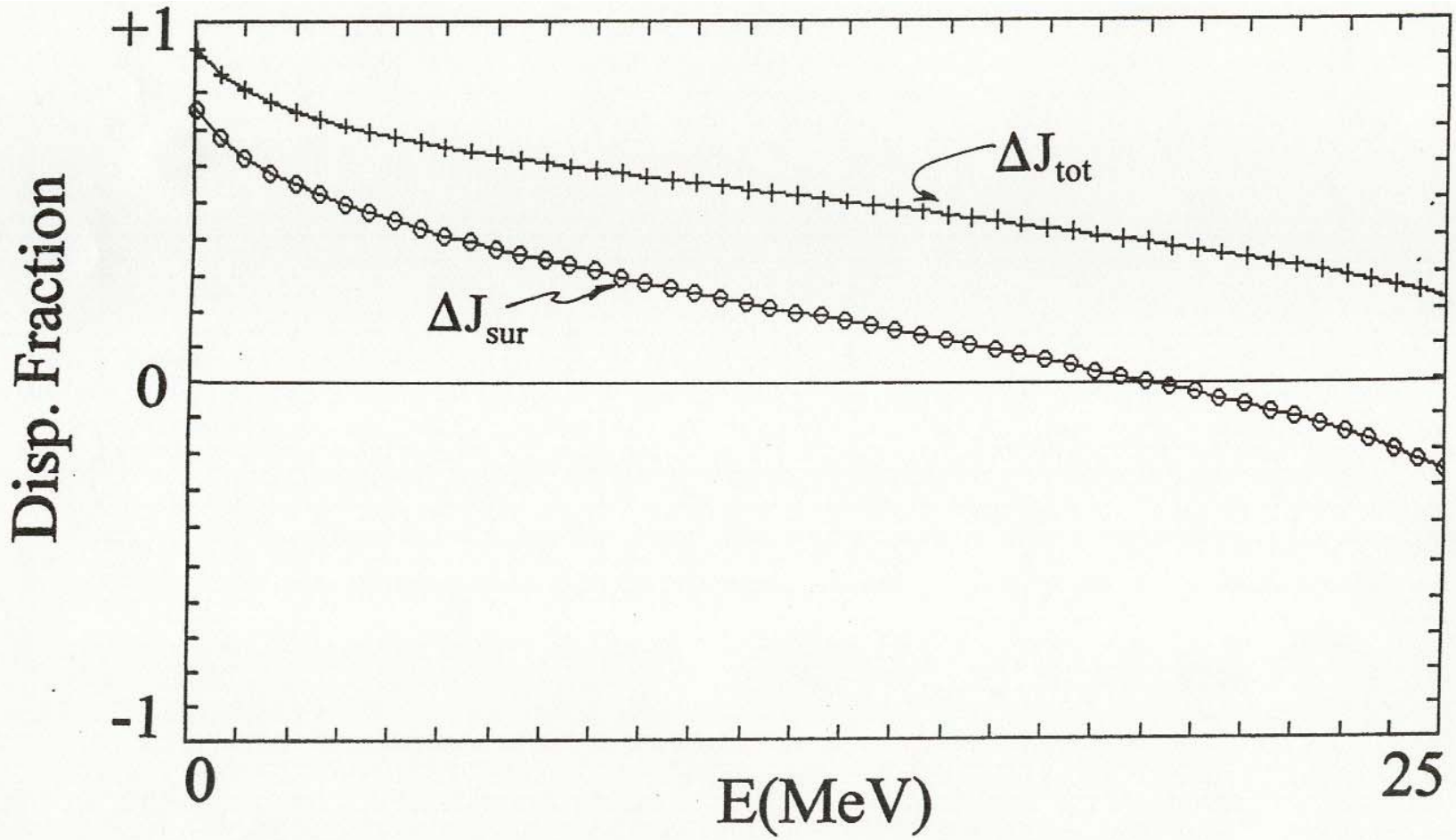

Fig. 3. Dispersive faction as discussed in the text. ΔJ_{sur} and ΔJ_{tot} denote the surface and total dispersive-ratio contributions.

Appendix, FORTRAN source listing

```
CCCCC  CALCULATION OF DISPERSION CONTRIBUTIONS FROM R. LAWSON FORMULAS.
CCCCD  OUTPUT DIRECTLY APPLICABLE TO ABAREX.
CCCCC  SIMPLE FORMULATION DESCRIBED IN TECHNICAL MEMO ABOVE.
CCCCC  PROVIDES TOTAL, SURFACE AND VOLUME INTEGRAL
CCCCC  OUTPUT ON FILE "OUT".
CCCCC  RUNS ON SIMPLE PC WITH LAHEY COMPILER.
CCCCC  ALSO RUNS ON VAX WORK STATION AND VAX CLUSTER.
CCCCC  SHOULD RUN ON ANY MODEST FACILITY WITH A FORTRAN-77 COMPILER.
      COMMON EF,E,EX,DELTA,EN,EV,FE
      DIMENSION H(3,1500),X(4,1500)
C     DIMENSIONED FOR 500 MESH POINTS
C     IF MORE MESH POINTS ARE DESIRED ENLARGE THE ABOVE DIMENSION
C     STATEMENT AND INCREASE 'NUM' (BELOW) CORRESPONDINGLY.
      NUM=1500
C     ALL ENERGIES ARE IN MEV. ALL STRENGTHS (J) ARE VOLUME-INTEGRALS-
C     PER-NUCLEON IN UNITS OF MEV-FM**3,
 1    FORMAT(' EF, ABS VALUE OF FERMI ENERGY (MEV), ZERO EXIT, (F12.6)')
 2    FORMAT(F12.6)
 3    FORMAT(' EN OF FIG. 1 OF TECH. NOTE IN MEV, (F12.6)')
 4    FORMAT(' EV OF FIG. 1 OF TECH. NOTE IN MEV, (F12.6)')
 5    FORMAT(' J0 OF FIG. 1 OF TECH. NOTE IN MEV-FM**3, (F12.6)')
 6    FORMAT(' JN OF FIG. 1 OF TECH. NOTE IN MEV-FM**3, (F12.6)')
 7    FORMAT(' JV OF FIG. 1 OF TECH. NOTE IN MEV-FM**3, (F12.6)')
 8    FORMAT(' E-START OF CALCULATION IN MEV, (F12.6)')
 9    FORMAT(' E-END OF CALCULATION IN MEV, (F12.6)')
C     E-START SHOULD BE LESS THEN E-END
 10   FORMAT(' DE, ENERGY INCREMENT OF THE CALCULATION IN MEV, (F12.6)')
 11   FORMAT(' TOTAL DISP ','EF,J0,JN,JV',4(2X,F8.3))
 20   FORMAT(' SURFACE DISP ','EF,J0,JN,JV',4(2X,F8.3))
 13   FORMAT(' TOTAL INTEGRAL')
 15   FORMAT(10E10.3)
 16   FORMAT(1H )
 17   FORMAT(' DELTA FOR POLES IN MEV, TYPICALLY 0.05 (F12.6)')
 18   FORMAT(' SURFACE INTEGRAL')
 19   FORMAT(' VOLUME INTEGRAL')
      OPEN(10,FILE='OUT',STATUS='NEW')
 100  CONTINUE
      NJ=1
      WRITE(*,1)
      READ(*,2)EF
      IF(EF.EQ.0.0)stop
      WRITE(*,3)
      READ(*,2)EN
      WRITE(*,4)
      READ(*,2)EV
      WRITE(*,5)
      READ(*,2)WJ0
      WRITE(*,6)
      READ(*,2)WJN
      SL=(WJN-WJ0)/EN
      WRITE(*,7)
      READ(*,2)WJV
      WRITE(*,17)
      READ(*,2)DELTA
      WRITE(*,8)
      READ(*,2)ESTART
      WRITE(*,9)
      READ(*,2)ESTOP
      WRITE(*,10)
      READ(*,2)DE
      SLMAX=(WJV-WJN)/(EV-EN)
      DO 200 JJ=1,NUM
      E=ESTART+FLOAT(JJ-1)*DE
      EE=ABS(E+EF)
      IF(EE.LE.EF)FE=WJ0*EE**2/EF**2
      IF(EE.GT.EF.AND.EE.LE.(EN+EF))FE=WJ0+SL*(EE-EF)
```

```
      IF(EE.GT.(EN+EF).AND.EE.LE.(EV+EF))FE=WJN+SLMAX*(EE-EF-EN)
      IF(EE.GT.(EV+EF))FE=WJV
      IF(ABS(FE).LT.1.E-6)FE=1.E-6
      CALL CHECK
      A=(WJ0/((EF**2)*3.14159))*(-.5*EF**2+EF*(2.*EF+EX)+((EX+EF)**2)*
     &ALOG(ABS(EX/(EF+EX))))
      B=(WJ0/((EF**2)*3.14159))*(.5*EF**2+EF*EX+((EX+EF)**2)*
     &ALOG(ABS((EF+EX)/(2.*EF+EX))))
      C=(1./3.14159)*((WJN-WJ0)+(WJ0+((WJN-WJ0)/EN)*EX)*
     &ALOG(ABS((EX-EN)/EX)))
      D=(1./3.14159)*((WJ0-WJN)+(WJ0+((2.*EF+EX)*(WJ0-WJN))/EN)*ALOG
     &(ABS((2.*EF+EX)/(2.*EF+EX+EN))))
      ESS=(WJN/(3.14159*(EN-EV)))*((EV-EN)+(EX-EV)*ALOG(ABS((EV-EX)/
     &(EN-EX))))
      EVV=(WJV/(3.14159*(EN-EV)))*((EN-EV)+(EN-EX)*ALOG(ABS((EV-EX)/
     &(EN-EX))))
      FSS=(WJN/(3.14159*(EV-EN)))*((EV-EN)+(2.*EF+EV+EX)*
     &ALOG(ABS((2.*EF+EN+EX)/(2.*EF+EV+EX))))
      FVV=(WJV/(3.14159*(EN-EV)))*((EV-EN)+(2.*EF+EN+EX)*
     &ALOG(ABS((2.*EF+EN+EX)/(2.*EF+EV+EX))))
      GH=(WJV/(3.14159))*ALOG(ABS((2.*EF+EV+EX)/(EV-EX)))
      FINT=A+B+C+D+ESS+EVV+FSS+FVV+GH
      FINS=A+B+C+D+ESS+FSS
      FINV=EVV+FVV+GH
      DISPT=FINT/FE
      IF(EX.GE.EV)GO TO 30
      DISPS=FINS/FE
      GO TO 31
30    DISPS=0.0
31    IF(E.GE.0.)GO TO 41
      DISPT=0.0
      DISPS=0.0
41    H(1,NJ)=EX
      H(2,NJ)=DISPT
      H(3,NJ)=DISPS
      X(1,NJ)=EX
      X(2,NJ)=FINT
      X(3,NJ)=FINS
      X(4,NJ)=FINV
      IF(E.GT.ESTOP)GO TO 35
      NJ=NJ+1
200   CONTINUE
35    NJ=NJ-1
      WRITE(10,11)EF,WJ0,WJN,WJV
      DO 40 J=1,NJ
      IF(H(1,J).LE.0.)GO TO 40
      WRITE(10,15)H(1,J),H(2,J)
40    CONTINUE
      WRITE(10,16)
      WRITE(10,20)EF,WJ0,WJN,WJV
      DO 42 J=1,NJ
      IF(H(1,J).LE.0.)GO TO 42
      WRITE(10,15)H(1,J),H(3,J)
42    CONTINUE
      WRITE(10,16)
      WRITE(10,13)
      DO 50 J=1,NJ
      WRITE(10,15)X(1,J),X(2,J)
50    CONTINUE
      WRITE(10,16)
      WRITE(10,18)
      DO 60 J=1,NJ
      WRITE(10,15)X(1,J),X(3,J)
60    CONTINUE
      WRITE(10,16)
      WRITE(10,19)
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```
      DO 70 J=1,NJ
      WRITE(10,15)X(1,J),X(4,J)
 70   CONTINUE
      WRITE(10,16)
      GO TO 100
      END
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      SUBROUTINE CHECK
      COMMON EF,E,EX,DELTA,EN,EV,FE
C GENERAL
      IF(FE.GT.0.0)GO TO 5
 6    FORMAT(' POTENTIAL=0 IS ILLEGAL')
      WRITE(*,6)
      STOP
 5    EX=E
      IF(EN.LT.EV)GO TO 1
 2    FORMAT('  ILLEGAL INPUT, STOP')
      WRITE(*,2)
      STOP
 1    IF(EF.NE.0.0)GO TO 3
 4    FORMAT('  ILLEGAL FERMI-E, STOP')
      WRITE(*,4)
      STOP
C A
 3    IF(ABS(EF+E).LE.DELTA.AND.E.GE.-EF)EX=-(EF-DELTA)
      IF(ABS(EF+E).LT.DELTA.AND.E.LE.-EF)EX=-(EF+DELTA)
      IF(ABS(E).LE.DELTA.AND.E.GE.0.)EX=DELTA
      IF(ABS(E).LE.DELTA.AND.E.LT.0.)EX=-DELTA
C B
      IF(ABS(E+EF).LE.DELTA.AND.E.GT.-EF)EX=-EF+DELTA
      IF(ABS(E+EF).LE.DELTA.AND.E.LE.-EF)EX=-EF-DELTA
      IF(ABS(E+2.0*EF).LE.DELTA.AND.E.GT.-(2.*EF))EX=-2.0*EF+DELTA
      IF(ABS(E+2.0*EF).LT.DELTA.AND.E.LE.-(2.*EF))EX=-2.0*EF-DELTA
C C
      IF(ABS(E-EN).LE.DELTA.AND.E.GT.EN)EX=EN+DELTA
      IF(ABS(E-EN).LT.DELTA.AND.E.LE.EN)EX=EN-DELTA
      IF(ABS(E).LE.DELTA.AND.E.GE.0.)EX=+DELTA
      IF(ABS(E).LE.DELTA.AND.E.LT.0.)EX=-DELTA
C D
      IF(ABS(E+2.*EF).LE.DELTA.AND.E.GT.(-2.*EF))EX=-2.*EF+DELTA
      IF(ABS(E+2.*EF).LT.DELTA.AND.E.LE.(-2.*EF))EX=-2.*EF-DELTA
      IF(ABS(E+(2.*EF+EN)).LE.DELTA.AND.E.GT.(-(2.*EF+EN)))EX=
     &-(2.*EF+EN)+DELTA
      IF(ABS(E+(2.*EF+EN)).LT.DELTA.AND.E.LE.(-(2.*EF+EN)))EX=
     &-(2.*EF+EN)-DELTA
C E-S
      IF(ABS(EN-E).LE.DELTA.AND.E.GT.EN)EX=EN+DELTA
      IF(ABS(EN-E).LE.DELTA.AND.E.LE.EN)EX=EN-DELTA
      IF(ABS(E-EV).LE.DELTA.AND.E.GT.EV)EX=EV+DELTA
      IF(ABS(E-EV).LT.DELTA.AND.E.LE.EV)EX=EV-DELTA
C E-V
      IF(ABS(EN-E).LE.DELTA.AND.E.GT.EN)EX=EN+DELTA
      IF(ABS(EN-E).LE.DELTA.AND.E.LE.EN)EX=EN-DELTA
      IF(ABS(E-EV).LE.DELTA.AND.E.GT.EV)EX=EV+DELTA
      IF(ABS(E-EV).LE.DELTA.AND.E.LE.EV)EX=EV-DELTA
C F-S
      IF(ABS((2.*EF+EN)+E).LE.DELTA.AND.E.GT.-(2.*EF+EN))EX=
     &-(2.*EF+EN)+DELTA
      IF(ABS((2.*EF+EN)+E).LE.DELTA.AND.E.LE.-(2.*EF+EN))EX=
     &-(2.*EF+EN)-DELTA
      IF(ABS((2.*EF+EV)+E).LE.DELTA.AND.E.GT.-(2.*EF+EV))EX=
     &-(2.*EF+EV)+DELTA
      IF(ABS((2.*EF+EV)+E).LT.DELTA.AND.E.LE.-(2.*EF+EV))EX=
     &-(2.*EF+EV)-DELTA

C F-V IF(ABS((2.*EF+EN)+E).LE.DELTA.AND.E.GT.-(2.*EF+EN))EX=
```

```
     &-(2.*EF+EN)+DELTA
      IF(ABS((2.*EF+EN)+E).LE.DELTA.AND.E.LE.-(2.*EF+EN))EX=
     &-(2.*EF+EN)-DELTA
      IF(ABS((2.*EF+EV)+E).LE.DELTA.AND.E.GT.-(2.*EF+EV))EX=
     &-(2.*EF+EV)+DELTA
      IF(ABS((2.*EF+EV)+E).LE.DELTA.AND.E.LE.-(2.*EF+EV))EX=
     &-(2.*EF+EV)-DELTA
C G+H
      IF(ABS(-(2.*EF+EV)-E).LE.DELTA.AND.E.GT.-(2.*EF+EV))EX=
     &-(2.*EF+EV)+DELTA
      IF(ABS(-(2.*EF+EV)-E).LE.DELTA.AND.E.LE.-(2.*EF+EV))EX=
     &-(2.*EF+EV)-DELTA
      IF(ABS(EV-E).LE.DELTA.AND.E.GT.EV)EX=EV+DELTA
      IF(ABS(EV-E).LT.DELTA.AND.E.LE.EV)EX=EV-DELTA
      RETURN
      END
```