**BINDING EFFECTS ON
REACTIVITY CHANGE FOR TRANSITIONS
FROM SOLID TO LIQUID PHASE
IN A FAST REACTOR SYSTEM**

R. E. SCHENTER AND A. G. GIBBS

APRIL 1968

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FROM SOLID TO LIQUID PHASE IN A FAST REACTOR SYSTEM

By

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ABSTRACT

The change in reactivity due to changes in the effective capture cross section of ^{238}U bound in a UO_2 lattice for transitions from solid to liquid phase is studied for a typical fast reactor system. Calculations indicate that this change in reactivity from the Doppler effect due to melting of UO_2 is negligible (less than 0.55 cent). It is assumed that at the high melting temperature and for a fast reactor flux, the binding effects can be well described in terms of a free gas model with an effective temperature. This "weak binding" or "short compound nucleus lifetime" approximation is carefully investigated.

TABLE OF CONTENTS

	ABSTRACT	iii
I.	INTRODUCTION	1
II.	ABSORPTION OF NEUTRONS BY BOUND NUCLEI	2
III.	WEAK BINDING OR SCNL (SHORT COMPOUND NUCLEUS LIFETIME) APPROXIMATION	4
IV.	EFFECTIVE TEMPERATURE MODEL AND THE DOPPLER COEFFICIENT	10
V.	CONCLUSIONS	11
	REFERENCES	12
	APPENDIX A - FOURIER TRANSFORMATION RELATIONS.	A.1
	APPENDIX B - PROGRAMS INSCNL AND SCNL.	B.1
	DISTRIBUTION	.Distr-1

BINDING EFFECTS ON REACTIVITY CHANGE FOR TRANSITIONS
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I. INTRODUCTION

The change in reactivity due to changes in the effective capture cross section for ^{238}U in a UO_2 lattice in going from a solid to liquid state could have importance for safety considerations in a fast reactor system, since during melting, the material temperature is constant, resulting in zero negative feedback from the normal Doppler effect. The negative change in reactivity from the normal feedback, an important safety mechanism for fast reactors, does not occur when the UO_2 is melting.

This report investigates the change in reactivity from the Doppler effect due to melting of the fuel in a typical fast reactor core. It is assumed that for the high melting temperature ($\sim 3000^\circ\text{K}$) and for the energies associated with a fast reactor flux, the binding effects can be well described in terms of a free gas model with an effective temperature. This assumption is equivalent to the "weak binding"⁽¹⁾ or "SCNL" (short compound nucleus lifetime)⁽²⁾ approximation. Physically, the SCNL approximation is reasonable for high temperatures and high neutron energies, since the relative velocities of neutrons and nuclei are then large. Thus interactions - if they are to occur at all - must take place in time intervals so short that the neutrons are aware only of the presence and velocities of the nuclei, and not of their accelerations.

Section II of this report outlines the general formalism for the absorption cross section of neutrons incident on bound target nuclei.

Section III develops an expression for the bound capture cross section in terms of an asymptotic series of which the first term represents the SCNL approximation. Graphical results are presented showing the validity of this approximation for several typical resonances at energies important for Doppler effect calculations. Section IV gives the results of reactivity calculations, where the effective temperature model (SCNL approximation) has been used for solid UO_2 . Section V summarizes the results of this study.

II. ABSORPTION OF NEUTRONS BY BOUND NUCLEI

If we consider the absorption of neutrons by a nucleus bound rigidly in place, the process is characterized by a cross section $\sigma_{ab}(E)$, where E is the laboratory energy of the incident neutron. (The cross section might be given, for example, by the single-level Breit-Wigner formula.) In problems of practical interest, however, the absorbing atom is not bound rigidly in place, but either recoils essentially freely, as in a gas, or is partially constrained through interactions with its neighbors, as in a liquid or crystal. In these cases, the momentum $\vec{p}$ of the incident neutron is transferred to the system of atoms of which the absorbing atom is a member. Some energy, say $\hbar\omega$, must also be transferred to the system when the absorbing atom recoils. Thus, only an energy $E - \hbar\omega$ is available for compound nucleus formation. To obtain an expression for the cross section in this case, we introduce a function $S(\vec{p}, \omega, T)$, which is defined to be the probability that an energy $\hbar\omega$ is transferred to the system when it absorbs momentum $\vec{p}$. Here T is the system temperature. Clearly, for an atom of a free gas the recoil energy and momentum transfer are related by $\hbar\omega = p^2/2M$, so that for a gas, $S(\vec{p}, \omega, T) = \delta(\omega - \frac{p^2}{2M\hbar})$. However, for a liquid or crystal, $S(\vec{p}, \omega, T)$ is a much more complicated function. For a given value of ω , absorption can take place if energy $\hbar\omega$ is transferred

to the scattering system while $E - \hbar\omega$ goes into compound nucleus formation. The probability for this to occur is clearly $\sigma_{ab}(E - \hbar\omega) S(\vec{p}, \omega, T)$. The cross section is obtained by summing the contributions for all ω .

The expression for the absorption cross section in the laboratory system is thus given by

$$\sigma_a(E, T) = \int_{-\infty}^{\infty} \sigma_{ab}(E - \hbar\omega) S(\vec{p}, \omega, T) d\omega. \quad (1)$$

For a nucleus bound in an isotropic harmonic crystal,[†] (3)

$$S(\vec{p}, \omega, T) = S(p, \omega, T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-it\omega} e^{\{(R/\hbar)[\gamma(t) - \gamma(0)]\}} \quad (2)$$

Here

$$R = \text{recoil energy} = \frac{m}{(M + m)} E, \quad (3)$$

$$\gamma(t) = \int_0^{\omega_{\max}} [\coth(\frac{\hbar\omega}{2kT}) \cos(\omega t) + i \sin(\omega t)] \frac{g(\omega)}{\omega} d\omega \quad (4)$$

$$\equiv \gamma_R(t) + i \gamma_I(t), \quad (5)$$

and $g(\omega)$ is the phonon frequency distribution function of the lattice. When the Fourier transform of $\sigma_{ab}(E)$ is introduced, $\phi(t)$, Equation (1) becomes (see Appendix IA)

$$\sigma_a(E, T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(t) e^{-i[Et - R\gamma_I(t)]/\hbar} e^{R[\gamma_R(t) - \gamma_R(0)]/\hbar} dt. \quad (6)$$

For the particular case of a single level Breit-Wigner form for $\sigma_{ab}(E)$,

$$\sigma_{ab}(E) = \frac{A_{\Gamma} E_0}{(E - E_0)^2 + \Gamma^2/4}, \quad (7)$$

[†] We will assume this to be true for ^{238}U in a UO_2 crystal.

$\phi(t)$ is given as (see Appendix IB)

$$\phi(t) = A_{\Gamma E_0} \frac{2\pi}{\Gamma \hbar} e^{iE_0 t/\hbar} e^{-(\Gamma/2)|t|/\hbar}, \quad (8)$$

and Equation (6) becomes

$$\sigma_a(E, T) = \frac{2A_{\Gamma E_0}}{\Gamma \hbar} \int_0^\infty e^{-(\Gamma/2)t/\hbar} + R[\gamma_R(t) - \gamma_R(0)]/\hbar, \\ \cos[(E - E_0)t/\hbar + R\gamma_I(t)/\hbar] dt. \quad (9)$$

The Breit-Wigner form given by Equation (9) will be used for the analyses in following sections, since to a good approximation, it represents the absorption cross in the energy region important for the Doppler effect.

III. WEAK BINDING OR SCNL (SHORT COMPOUND NUCLEUS LIFETIME) APPROXIMATION

To examine the validity of the SCNL approximation for high melting temperatures (~ 3000 °K) and resonances at energies that are important for Doppler coefficient analyses in a typical fast reactor, we use an asymptotic expansion for the absorption cross section⁽³⁾ that gives as its first term the SCNL approximation.

To obtain the asymptotic expansion, the power series expansions of $\gamma_R(t)$ and $\gamma_I(t)$ are used, which from Equations (4) and (5) are given as

$$\gamma_R(t) = \gamma_R(0) - \gamma_2 t^2 + \gamma_4 t^4 - \gamma_6 t^6 + \dots \quad (10)$$

$$\gamma_I(t) = t - \frac{1}{3!} \langle \omega^2 \rangle t^3 + \frac{1}{5!} \langle \omega^4 \rangle t^5 + \dots, \quad (11)$$

where

$$\gamma_n = \int_0^{\omega_{\max}} \coth\left(\frac{\hbar\omega}{2kT}\right) \frac{g(\omega)}{\omega} \frac{\omega^n}{n!} d\omega, \quad (12)$$

$$\langle \omega^n \rangle = \int_0^{\omega_{\max}} \omega^n g(\omega) d\omega. \quad (13)$$

Substitution of Equations (10) and (11) into Equation (9) gives

$$\sigma_a(E, T) = \frac{2A_{\Gamma E_O}}{\Gamma} \int_0^\infty e^{-(\Gamma/2)y - \Delta^2 y^2} \cos[(E_O - E + R)y + R(W_1 y^3 + W_2 y^5 + \dots) e^{R(G_2 y^4 + G_3 y^6 + \dots)}] dy, \quad (14)$$

where

$$\Delta = (4RKT_{\text{eff}})^{1/2} = \text{"effective Doppler width"}, \quad (15)$$

$$KT_{\text{eff}} = -G_1 = \text{the average energy per mode of oscillation}, \quad (16)$$

$$W_n = (-1)^n \hbar^{2n} \langle \omega^{2n} \rangle / (2n+1)!, \quad (17)$$

and

$$G_n = (-1)^n \hbar^{2n-1} \gamma_{2n}. \quad (18)$$

Expanding the cosine and second exponential term in Equation (14) gives

$$\begin{aligned} \sigma_a(E, T) = \sigma_a(E, T)_{\text{SCNL}} + \frac{2A_{\Gamma E_O}}{\Gamma} R \int_0^\infty y^3 e^{-(\Gamma/2)y - \Delta^2 y^2} \\ \{ \cos(E - E_O + R)y [G_2 y + (G_3 - RW_1^2/2)y^3 + \dots] \\ - \sin(E - E_O + R)y (W_1 + W_2 y^2 + \dots) \} dy, \end{aligned} \quad (19)$$

where

$$\sigma_a(E, T)_{\text{SCNL}} = \frac{2A_{\Gamma E_O}}{\Gamma} \int_0^\infty e^{-(\Gamma/2)y - \Delta^2 y^2} \cos(E - E_O + R)y dy \quad (20)$$

is the SCNL approximation expression for the absorption cross section.

This expression is equivalent to that which would be given for the absorption of particles by free gas targets having a temperature T_{eff} . The range of validity of the SCNL approximation is usually expressed by the following inequality:^(1,2)

$$\Gamma/2 + \Delta/2 \gg \hbar\omega_{\text{max}}. \quad (21)$$

The above inequality is a statement that the maximum relaxation period of the lattice, $1/\omega_{\text{max}}$, is large in comparison with the compound nucleus lifetime, $\hbar/[\Gamma/2 + \Delta/2]$.

To look at the validity of the SCNL approximation in detail, we compared the SCNL model, a free gas model, and an exact calculation using Equation (19).

Figures 1, 2, 3, and 4 show these results⁺ for resonances of energies 2.0, 1.0, and 0.1 keV.⁺⁺ In Figure 1 the full absorption curve is given, where the small rectangle at the peak of the curve represents the region of interest. This region is reproduced in detail in Figures 2, 3, and 4. Figures 2 and 3 illustrate the main point to be made in this section, that the SCNL approximation cross section is very close in value to the "exact" cross section for resonances with energies important in Doppler effect calculations for fast reactor systems.⁺ The

⁺ The values plotted on the curves given in Figures 1, 2, 3, and 4 were obtained using Programs INSCNL and SCNL (listings are given in Appendix B). The "exact" cross section curve was generated by summing terms indicated in the series given by Equation (19). The convergence of this series was rapid for energies and temperature considered in this section. The phonon distribution (Figure 5) given by Dolling et al. (Reference 4) was used for all calculations.

⁺⁺ The resonances picked are not specific resonances of ^{238}U but represent typical resonances of ^{238}U with the exception that minimum natural width (Γ) values were used so as to validate the SCNL approximation for cases with the strongest binding effects.

⁺ Essentially 99% of the Doppler effect of ^{238}U comes from the broadening of resonances with energies of 0.1 keV or more. See Reference 5 for a discussion of this point.

FIGURE 1. Absorption Cross Section of ^{238}U Bound in a UO_2 Crystal ($E_0 = 1 \text{ keV}$, $T = 3000 \text{ }^\circ\text{K}$), Dolling Model

FIGURE 2. Absorption Cross Section of ^{238}U Bound in a UO_2 Crystal ($E_0 = 1 \text{ keV}$, $T = 3000 \text{ }^\circ\text{K}$), Dolling Model

FIGURE 3. Absorption Cross Section of ^{238}U Bound in a UO_2 Crystal ($E_0 = 2 \text{ keV}$, $T = 3000 \text{ }^\circ\text{K}$), Dolling Model

FIGURE 4. Absorption Cross Section of ^{238}U Bound in a UO_2 Crystal ($E_0 = .1 \text{ keV}$, $T = 3000 \text{ }^\circ\text{K}$), Dolling Model

FIGURE 5. *Dolling Phonon Distribution for ^{238}U in a UO_2 Lattice*

"free gas" curves shown in Figures 2, 3, and 4 represent the absorption cross section for unbound targets having an average kinetic energy corresponding to the actual material temperature. In Figure 4 results are given for a resonance with an energy at the lower boundary of the Doppler effect region. At this energy, it is seen that SCNL approximation is of questionable accuracy.

In Table I the range of the parameter α , which is the ratio of the maximum relaxation period of the lattice to compound nucleus lifetime,

$$\alpha \equiv (\Gamma/2 + \Delta/2)/\hbar\omega_{\text{max}}, \quad (22)$$

is given for the energy regions considered in Figures 2, 3, and 4. An examination of Table I together with these figures[†] indicates quantitatively the validity of the SCNL approximation as expressed by the inequality Expression (21).

TABLE I. *Range of α Values for the Resonances of ^{238}U ($T = 3000^\circ\text{K}$)*

<u>E, keV</u>	<u>α_{Min}</u>	<u>α_{Max}</u>
E $\sim$ 0.1	4	6
E $\sim$ 1.0	13	15
E $\sim$ 2.0	17	20

IV. EFFECTIVE TEMPERATURE MODEL AND THE DOPPLER COEFFICIENT

The change in reactivity from the Doppler effect for a change in state in the UO_2 lattice is estimated in this section. First, it is assumed that in the liquid state the strong binding effects are lost so that the ^{238}U atoms absorb as if they were in a free gas state at the temperature of the liquid. This will give an upper bound to the calculated change in reactivity for the solid to liquid change. Second, from the results of the previous section the solid state is well represented in terms of a free gas model with an effective temperature (SCNL-approximation). Therefore, the expression for the change in reactivity is simply

$$\delta k_{\text{solid} \rightarrow \text{liquid}} \leq k(T_{\text{eff}}) - k(T), \quad (23)$$

where $k(T)$ is the multiplication factor of a fast reactor system with the usual assumption that the ^{238}U atoms absorb as a free gas at a temperature T .

[†] The α values for the resonances given in Figures 2, 3, and 4 are the lowest ones in their respective ranges (α equals 4 for the 0.1 keV resonance in Figure 4, for example).

The change in reactivity, δk , of Equation (23) has been calculated for typical fast reactor cores using Program FCC⁽⁶⁾ for material temperatures of 3000 °K. The effective temperature calculated from Equations (12), (16), and (18) by Program INSCNL (Appendix B) is found to be 3008 °K for the Dolling phonon distribution. With the above, δk was found to be positive but less than 1.65×10^{-5} ,[†] which corresponds to a reactivity change of less than .55 cent for a typical fast reactor core.

V. CONCLUSIONS

The results given in Section III indicate that for the high melting temperature and the energies associated with a fast reactor flux, the absorption process by ^{238}U targets in a crystalline state can, to a good approximation, be described in terms of a free gas model with an effective temperature. With this, an upper bound to the change in reactivity due to melting can be easily calculated [Equation (23)]. This value, which is given in Section IV, though positive, is quite small (≈ 0.55 cent). Consequently, the Doppler effect due to melting does not give significant reactivity feedback and the usual assumption of neglecting its effect is well justified.

[†] It is interesting to note that the change in reactivity given by Expression (23) occurs with no change in material temperature T , which implies an infinite value for the Doppler coefficient $(\frac{1}{T} \frac{dk}{dT})$ at the melting temperature.

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APPENDIX A

FOURIER TRANSFORMATION RELATIONS

APPENDIX A
FOURIER TRANSFORMATION RELATIONS

A.1. GENERAL CASE

The Fourier transform of $\sigma_{ab}(E)$, $\phi(t)$, is defined as

$$\phi(t) \equiv \frac{1}{\hbar} \int_{-\infty}^{\infty} \sigma_{ab}(E) e^{iEt/\hbar} dE. \quad (A-1)$$

The cross section $\sigma_{ab}(E)$ is then given in terms of $\phi(t)$ as

$$\sigma_{ab}(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(t) e^{-iEt/\hbar} dt. \quad (A-2)$$

Substituting Equations (A-2), (4), (2) into Equation (1) gives

$$\begin{aligned} \sigma_a(E, T) &= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(t') e^{-i(E - \hbar\omega)t'/\hbar} e^{-it\omega} \\ &\quad e^{iR\gamma_I(t)/\hbar} e^{[R(\gamma_R(t) - \gamma_R(0))]/\hbar} dt dt' d\omega \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t' - t)} d\omega \right\} \phi(t') e^{-iEt'/\hbar} \\ &\quad e^{iR\gamma_I(t)/\hbar} e^{R[\gamma_R(t) - \gamma_R(0)]/\hbar} dt dt' \end{aligned}$$

Since

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t - t')} d\omega,$$

$$\sigma_a(E, T) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(t) e^{-i[Et - R\gamma_I(t)]/\hbar} e^{R[\gamma_R(t) - \gamma_R(0)]/\hbar} dt. \quad (A-3)$$

A.2. SINGLE LEVEL BREIT-WIGNER FORM

With the following form for $\sigma_{ab}(E)$:

$$\sigma_{ab}(E) = \frac{A_{\Gamma} E_0}{(E - E_0)^2 + \Gamma^2/4}, \quad (A-4)$$

$\phi(t)$ is given as

$$\begin{aligned}
 \phi(t) &= \frac{A_{\Gamma E_0}}{\hbar} \int_{-\infty}^{\infty} \frac{e^{iEt/\hbar} dE}{(E - E_0)^2 + \Gamma^2/4} = \frac{A_{\Gamma E_0}}{\hbar} \int_{-\infty}^{\infty} \frac{1}{x^2 + \Gamma^2/4} \\
 &\quad e^{i(x+E_0)t/\hbar} dx \\
 &= \frac{A_{\Gamma E_0}}{\hbar} e^{iE_0 t/\hbar} \int_{-\infty}^{\infty} \frac{e^{ixt/\hbar}}{(x^2 + \Gamma^2/4)} = \frac{|t|}{t} \frac{1}{\hbar} e^{iE_0 t/\hbar} 2\pi i \\
 &\quad \text{Res}(x = \frac{|t|}{t} i\Gamma/2) \\
 &= A_{\Gamma E_0} \frac{2\pi}{\hbar\Gamma} e^{iE_0 t/\hbar} e^{-\Gamma|t|/2\hbar}.
 \end{aligned}
 \tag{A-5}$$

APPENDIX B

A LISTING OF PROGRAMS INSCNL AND SCNL


```

                                SCNL
C   PROGRAM SCNL CALCULATES THE ABSORPTION CROSS SECTION FOR NEUTRONS INCIDENT
C   ON NUCLEI BOUND IN A CRYSTAL LATTICE
-IT FOR MAIN,MAIN
  11 FORMAT(6E12.5)
  12 FORMAT (12I5)
  13 FORMAT (I3,8E14.7)
  15 FORMAT(6E12.5)
  DIMENSION GT(20),W(20),GTT(1,20),TT(10),S(41),II(10),GFT(20)
  READ(5,12) NW,NT,K1
  READ(5,15) (W(N),N=1,NW)
  WRITE(6,15) (W(N),N=1,NW)
  DO 2 N=1,NT
  READ(5,15) TT(N),(GTT(N,M),M=1,NW)
  2 WRITE (6,15) TT(N),(GTT(N,M), M=1,NW)
  N1=301
  CALL SETEOF($310)
  1 READ(5,11)GAM,EB,A
  WRITE(6,11)GAM,EB,A
  READ(5,12)(II(N),N=1,10)
  N=1
  3 I=II(N)
  WRITE(6,11)TT(I)
  GFT(1)=-TT(I)
  E=EB-GAM*(K1-1)/20.
  DO 6 J=1,NW
  6 GT(J)=GTT(I,J)
  MM=-(K1-1)/2
  DO 4 M=1,K1
  S(1)=SCNL(GAM,GFT,W,A,EB,E,N1,1)
  DO 5 J=1,4
  M1=J+1
  5 S( M1)=SCNL(GAM,GT,W,A,EB,E,N1,J )
  WRITE(6,13)MM,E,(S(J),J=1,7)
  MM=MM+1
  4 E=E+GAM/10.
  N=N+1
  IF(II(N))3,1,3
  310 CONTINUE
  CALL EXIT
  END
-IT FOR SCNL,SCNL
  FUNCTION SCNL(GAM,GT,W,A,EB,E,N1,M1)
  DIMENSION GT(1),W(1),GG(20)
  YMAX=SQRT(3600./(-GT(1)*EB))
  DEL=YMAX/N1
  R=E/(A+1.)

```

```

Y1=(EB-E)*(1.+1./A)
GG(2)=W(1)
GG(3)=GT(2)
GG(4)=W(2)
GG(5)=-.5*R*W(1)**2+GT(3)
GG(6)=W(3)+R*W(1)*GT(2)
GG(7)=-R*W(1)*W(2)+GT(4)
S=.5
DO 1 N=1,N1
Y=N*DEL
Z=Y
X1=1./R
X2=0.
    IF(M1.EQ.1) GO TO 1
DO 2 L=2,M1
M=2*L-2
Z=Z*Y**2
    X2=X2+GG(M)*Z
2 X1=X1+GG(M+1)*Z*Y
1 S=S+EXP(-GAM*Y/2.+R*GT(1)*Y*Y)*R*(X1*COS(Y1*Y)-X2*SIN(Y1*Y))
SCNL=S*DEL
RETURN
END
- XQT MAIN

```

B.2

BNWL-717

```

                                INSCNL
C  INSCNL CALCULATES INPUT FOR PROGRAM SCNL IN PUNCHED CARD FORM FOR A GIVEN
C  PHONON DISTRIBUTION
-IT FOR MAIN,MAIN
  11 FORMAT (3E14.8)
  12 FORMAT (12I5)
  15 FORMAT(6E12.5)
    DIMENSION G(500),GT(20),W(20),X(500),F(500),CC(40)
    READ(5,12)N1,M1
    WRITE (6,12)N1,M1
    A = .5* .0041355
C  STORE G(N) FOR N=1,N1 WHERE SUM X(N)*G(N)=1,INCLUDE HWMAX
C
    M2=2*M1+1
    CC(1)=1.
    DO 5 N=2,M2
  5  CC(N)=N*CC(N-1)
    H=HWMAX/(N1-1)
    DO 1 N=1,N1
    X(N)=(N-1)*H
  1  F(N)=G(N)
    C = SNT(G,X,N1)
    WRITE(6,11)C
    DO 2 M=1,M1
    DO 3 N=1,N1
    Z=X(N)**2
  3  F(N)=F(N)*Z
  2  W(M)=SNT(F,X,N1)*(-1)**M/(CC(2*M+1)*C)
    PUNCH 15,(W(M),M=1,M1)
    CALL SETEOF($310)
  8  READ (5,15) T
    F(1)=G(1)*2*T
    DO 4 N=2,N1
  4  F(N)=(X(N)*G(N))/(TANH(X(N)/(2*T)) )
    GT(1)=-SNT(F,X,N1)/(2.*C)
    DO 9 M=2,M1
    DO 10 N=1,N1
    Z=X(N)**2
  10 F(N)=Z*F(N)
  9  GT(M)=(-1)**M*SNT(F,X,N1)/(CC(2*M)*C)
    PUNCH 15,T,(GT(N),N=1,M1)
    GO TO 8
310 CONTINUE
    CALL EXIT
    END

```


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