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EFFECT OF ANISOTROPIC SCATTERING ON CRITICAL-MASS CALCULATIONS

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ABSTRACT

Formulas are developed to include the effect of anisotropic scattering in critical-mass calculations by the spherical-harmonic method. These are applied to the specific case of a 25 core surrounded by an infinite tungsten carbide tamper. The results of the calculations were found to be identical with those obtained by using the transport cross section wherever equations derived on the isotropic assumption indicated the total cross section should appear. By arguments based on the numerical results it is shown that the use of the transport cross section throughout will also be an extremely good approximation when we have multiplying media.

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EFFECT OF ANISOTROPIC SCATTERING ON CRITICAL-MASS CALCULATIONS

This report gives the results of some investigations concerning the effect of anisotropic scattering on critical-mass calculations in the one-velocity-group approximation. Until the advent of the S.H.M. (spherical-harmonic method) it had been impossible to solve critical-mass problems exactly with the inclusion of anisotropic scattering. The recipe had been given, though, and more or less justified, that the proper way to take this phenomenon into account was to use the transport cross section wherever formulas derived assuming isotropic scattering had the total cross section occurring. Using the S.H.M. it has proved possible to test the validity of the recipe by giving an exact solution, including anisotropy, in the case of a 25 core surrounded by a WC tamper. It is believed that this case is sufficiently typical to warrant a general conclusion about the recipe for all interesting cases. Actually, numerical calculations were made only for the critical case. However, by examining the results obtained it is easy to draw inferences in the case of other multiplication rates. The problem was done in P_3 rather than in a higher approximation, since it is known that for the ratio of tamper to core cross sections considered, P_3 gives a result accurate to about 1-1/2 percent. Moreover, the primary aim was to see the relative results of the transport recipe and the accurate solution, rather than to obtain an absolute figure.

In taking into account anisotropic scattering a procedure completely analogous to the ordinary application of the S.H.M. is followed. The Boltzmann equation is written in the form

$$\frac{\partial n}{\partial t} + \mu \frac{\partial n}{\partial r} + \frac{(1-\mu^2)}{r} \frac{\partial n}{\partial \mu} = -\sigma_t n + \int_{-1}^{1} n(r,\mu')d\mu' \int_{0}^{2\pi} \frac{\sigma_s}{2\pi} d\phi' + \frac{\nu\sigma_f}{2} \int_{-1}^{1} n(r,\mu')d\mu' \qquad (1)$$

where n is the neutron density as a function of position and velocity; σ_t is the total cross section per unit volume; $\sigma_s(\alpha)$ is the cross section per unit volume for scattering a neutron through an angle α per $d(\cos\alpha)$. μ is defined as $\cos\theta$, where θ is the angle between velocity and radius vectors. Symbols used for other cross sections per unit volume are: σ_f, fission; σ_{tr}, transport; σ_r, capture; σ_i, inelastic scattering; σ_e, elastic scattering. Without primes these quantities refer to the core; with primes, they refer to the tamper. It should be noted that the dimension of the foregoing cross sections is reciprocal length, and that these cross sections equal the cross section usually given in experimental papers multiplied by N, where N is the number of atoms per unit volume.

Expand σ_s so that:

$\sigma_s(\alpha) = \sum_{\ell=0}^{\infty}\left[(2\ell+1)/2\right]\sigma_\ell P_\ell(\cos\alpha)$, where the σ_ℓ's are constants. Let θ' be the angle which the velocity vector makes with the radius vector before collision and θ be the angle after collision. Similarly ϕ' and ϕ are the azimuthal angles before and after collision.

Then: $\cos\alpha = \mu\mu' - \sqrt{\mu^2 - 1}\,\sqrt{\mu'^2 - 1}\,\cos\omega$ (2)

where $\mu = \cos\theta$, $\mu' = \cos\theta'$, $\omega = \phi - \phi'$.

With this change of variable:

$$\int_0^{2\pi} \frac{\sigma_s(\alpha)}{2\pi}\, d\phi = \int_{\phi}^{\phi + 2\pi} \frac{\sigma_s}{2\pi}\, d\omega$$

The addition theorem for Legendre polynomials tells us that, if

$$Z = X X' - \sqrt{X^2 - 1}\,\sqrt{X'^2 - 1}\,\cos\omega$$

then

$$P_n(Z) = P_n(X)\, P_n(X') + 2\sum_{m=1}^{\infty} (-1)^m \frac{\Gamma(n-m+1)}{\Gamma(n+m+1)} P_n^m(X)\, P_n^m(X') \cos m\omega \qquad (3)$$

Hence

$$\int_{\phi}^{2\pi+\phi} P_n(\cos\alpha)\, d\omega = 2\pi\, P_n(\mu)\, P_n(\mu')$$

and

$$\int_0^{2\pi} \frac{\sigma_s(\alpha)}{2\pi}\, d\phi' = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2}\, \sigma_\ell\, P_\ell(\mu)\, P_\ell(\mu') \tag{4}$$

With this simplification (3) becomes:

$$\frac{\partial n}{\partial t} + \mu\frac{\partial n}{\partial r} + \frac{(1-\mu^2)}{r}\frac{\partial n}{\partial \mu} = -\sigma_t n + \int_{-1}^{1} n(r,\mu') \sum_0^{\infty} \frac{2\ell+1}{2}\, \sigma_\ell P_\ell(\mu) P_\ell(\mu')\, d\mu' + \frac{\nu\sigma_f}{2}\int_{-1}^{1} n\, d\mu' \tag{5}$$

Assume a time dependence of the form $n \sim e^{\gamma\sigma_{tr}t}$ (actually our form is $e^{\gamma\sigma_{tr}vt}$ but time units have been taken so that $v = 1$). Substituting this time dependence, cancelling factors of $e^{\gamma\sigma_{tr}t}$, and introducing $n = \sum_0^{\infty}\left[(2\ell+1)/(2)\right] n_\ell(r)\, P_\ell(\mu)$, Eq. (5) becomes:

$$\mu\sum_{\ell=0}^{\infty}\frac{dn_\ell}{dr} P_\ell(\mu) + \frac{(1-\mu^2)}{r}\sum_0^{\infty} n_\ell(r)\frac{dP_\ell}{d\mu} + (\sigma_t + \gamma\sigma_{tr})\sum_0^{\infty} n_\ell P_\ell = \frac{\nu\sigma_f n_0}{2} + \sum_0^{\infty}\frac{2\ell+1}{2}\,\sigma_\ell n_\ell P_\ell(\mu) \tag{6}$$

Multiplying by $P_\ell(\mu)d\mu$ and integrating from -1 to +1 there results the infinite set of differential equations:

$$\frac{1}{2\ell+1}\left[\ell n'_{\ell-1} + (\ell+1)n'_{\ell+1}\right] + \frac{1}{2\ell+1}\left[\frac{(\ell+1)(\ell+2)n_{\ell+1}}{r} - \frac{\ell(\ell-1)n_{\ell-1}}{r}\right] + (\sigma_t + \gamma - \sigma_\ell)n_\ell = \nu\sigma_f\, n_0\, \delta_{0\ell} \tag{7}$$

where $\delta_{0\ell}$ is the Kronecker delta.

For our purposes P_3 is sufficient and so we break off the set at $\ell = 3$. (When the set is broken off at ℓ_0, it is called the P_{ℓ_0} approximation.) This gives for the equations:

$$
\begin{aligned}
\ell = 0 \quad & n_1' + (2n_1/r) + \alpha_0 n_0 = 0 \\
\ell = 1 \quad & n_0' + 2n_2' + (6n_2/r) + 3\alpha_1 n_1 = 0 \\
\ell = 2 \quad & 2n_1' + 3n_3' + (12n_3/r) - (2n_1/r) + 5\alpha_2 n_2 = 0 \\
\ell = 3 \quad & 3n_2' - (6n_2/r) + 7\alpha_3 n_3 = 0
\end{aligned} \tag{8}
$$

For convenience in comparing our results with calculations not explicitly including anisotropy we will choose our units so that $(\sigma_{tr})_{core} = 1$. In these units we have for the core:

$$\alpha_0 = \sigma_t + \gamma - \sigma_0 - \nu\sigma_f$$

$$\alpha_i = \sigma_t + \gamma - \sigma_\ell \qquad \ell = 1, 2, 3.$$

Similar equations hold for the tamper where:

$$\alpha_i' = \sigma_t' + \gamma - \sigma_\ell' ; \qquad \ell = 0, 1, 2, 3.$$

It is interesting to note that the transport recipe leads to exactly the same equations but with α's having the following values:

$$\alpha_0 = \gamma - f \qquad\qquad \alpha_0' = \gamma - f'\sigma_{tr}'$$

$$\alpha_i = \gamma + 1,\ i = 1, 2, 3. \quad \alpha_i' = \gamma + \sigma_{tr}'$$

where f is $\left((\nu-1)\sigma_f - \sigma_r\right)/\sigma_{tr}$, and ν = number of neutrons emitted per fission. Thus very little additional complication is introduced by taking anisotropy into account. (In actually applying the recipe it is customary to start with the Boltzmann equation in a form that can be obtained from (1) by the substitution of σ_{tr} for σ_t, zero for σ_s, and $\sigma_{tr}(1+f)$ for $\nu\sigma_f$.)

The amount of anisotropy and the form of σ_s in the core and tamper may be seen in Figs. 1 and 2. These curves were determined as follows: for 25 the

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form was taken to correspond as closely as possible with experimental values at about 600 kev. The curve was then normalized to give an elastic transport cross section of 3.75 barns - determined by Serber and Rarita to be the likely one-velocity-group value. Other constants of 25 employed were: $\sigma_f = 1.56$ barns x N, $\sigma_i = 0.15$ barns x N, $\sigma_r = 0.15$ barns x N. These give an f of 0.39. The inelastic cross section was treated as an additional spherically symmetric contribution to the elastic scattering cross section. In the tamper the cross sections were due to contributions from W and C. The W was treated in exactly the same way as the 25 - normalizing $(\sigma_{elastic})_{transport}$ to 3.79 barns x N. For carbon, spherically symmetric scattering in the center-of-gravity system was assumed. This seems a fairly reasonable assumption and gives a curve that, although not fitting very closely to Manley's experimental values, does lie within the limits of error of the experimental points. For the WC, σ_i was taken as 0.78 barns x N and treated as spherically symmetric elastic. σ_r was 0.23 barns x N, giving an f' of -0.03. After determining these constants all cross sections were converted to units such that $\sigma_{tr}(25)$(which was 5.61 barns x N) had the value unity. ν was taken as 2.5.

Using these figures and fitting the σ_s curves as well as possible the following values are obtained for the coefficients σ_2 (in barns x N).

$$\sigma_0 = 5.05 \qquad \sigma_0' = 7.96$$

$$\sigma_1 = 1.153 \qquad \sigma_1' = 0.611$$

$$\sigma_2 = 0.444 \qquad \sigma_2' = 0.277$$

$$\sigma_3 = 0.0992 \qquad \sigma_3' = -0.0598$$

Solving our differential equations subject to the requirements of finiteness at the origin and vanishing at infinity we obtain: (where A_1, A_2, B_1, B_2 are constants still to be determined).

Core:

$$n_o = (A_1 \sin k_1 r + A_2 \sinh k_2 r)/r$$

$$n_1 = \alpha_o A_1\left[\frac{\cos k_1 r}{k_1 r} - \frac{\sin k_1 r}{k_1^2 r^2}\right] - \alpha_o A_2\left[\frac{\cosh k_2 r}{k_2 r} - \frac{\sinh k_2 r}{k_2^2 r^2}\right]$$

$$n_2 = \frac{c_1}{2} A_1\left[\left(\frac{1}{r} - \frac{3}{k_1^2 r^2}\right) \sin k_1 r + \frac{3 \cos k_1 r}{k_1 r^2}\right]$$

$$+ \frac{c_3}{2} A_2\left[\left(\frac{1}{r} + \frac{3}{k_2^2 r^3}\right) \sinh k_2 r - \frac{3 \cosh k_2 r}{k_2 r^2}\right]$$

$$n_3 = c_2 A_1\left[\left(\frac{2}{k_1^2 r^2} - \frac{5}{k_1^4 r^4}\right) \sin k_1 r - \left(\frac{1}{3 k_1 r} - \frac{5}{k_1^3 r^3}\right) \cos k_1 r\right]$$

$$+ c_4 A_2\left[\left(\frac{1}{3 k_2 r} + \frac{5}{k_2^3 r^3}\right) \cosh k_2 r - \left(\frac{2}{k_2^2 r^2} + \frac{5}{k_2^4 r^4}\right) \sinh k_2 r\right]$$

Tamper:

$$n_o = (B_1 e^{-v_1 r} + B_2 e^{-v_2 r})/r$$

$$n_1 = \alpha_o' B_1 e^{-v_1 r} \left(\frac{1}{v_1 r} + \frac{1}{v_1^2 r^2}\right) + \alpha_o' B_2 e^{-v_2 r} \left(\frac{1}{v_2 r} + \frac{1}{v_2^2 r^2}\right)$$

$$n_2 = \frac{c_5 B_1}{2} e^{-v_1 r}\left(\frac{1}{r} + \frac{3}{v_1 r^2} + \frac{3}{v_1^2 r^3}\right) + \frac{c_7}{2} B_2 e^{-v_2 r}\left(\frac{1}{r} + \frac{3}{v_2 r^2} + \frac{3}{v_2^2 r^3}\right)$$

$$n_3 = c_6 B_1 e^{-v_1 r} \left(\frac{1}{3 v_1 r} + \frac{2}{v_1^2 r^2} + \frac{5}{v_1^3 r^3} + \frac{5}{v_1^4 r^4}\right)$$

$$+ c_8 B_2 e^{-v_2 r} \left(\frac{1}{3 v_2 r} + \frac{2}{v_2^2 r^2} + \frac{5}{v_2^3 r^3} + \frac{5}{v_2^4 r^4}\right)$$

where:

$$c_1 = -\left[1 + \left((3\alpha_o \alpha_1)/(k_1^2)\right)\right]; \qquad c_2 = 2\alpha_o - (5/2)\alpha_2 c_1$$

$$c_3 = \left[\left((3\alpha_o \alpha_1)/(k_2^2)\right) - 1\right]; \qquad c_4 = 2\alpha_o - (5/2)\alpha_2 c_3$$

$$c_5 = \left[(3\alpha_o' \alpha_1')/(v_1^2) - 1\right]; \qquad c_6 = -\left[2\alpha_o' - (5/2)\alpha_2' c_5\right]$$

$$c_7 = \left[\left((3\alpha_o' \alpha_1')/(v_2^2)\right) - 1\right]; \qquad c_8 = -\left[2\alpha_o' - (5/2)\alpha_2' c_7\right]$$

(9)

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k_1 is the absolute value of the imaginary root, and k_2 is the positive, real root, of: $k^4 - \left[3\ \alpha_0 \alpha_1 + (28/9)\ \alpha_0\ \alpha_3 + (35/9)\ \alpha_2\ \alpha_3\right] k^2 + (35/3)\ \alpha_0 \alpha_1 \alpha_2 \alpha_3 = 0$

v_1 and v_2 are the positive, real roots of:

$$v^4 - \left[3\ \alpha_0' \alpha_1' + (28/9)\ \alpha_0'\ \alpha_3' + (35/9)\ \alpha_2'\ \alpha_3'\right] v^2 + (35/3)\ \alpha_0' \alpha_1' \alpha_2' \alpha_3' = 0.$$

Equating the n_ℓ's of core and tamper at $r = a$ (a is the radius of the core) gives four homogeneous equations for the A's and B's. The condition that these equations have a nontrivial solution is expressed by setting the determinant of the coefficients equal to zero. This, for specified γ, gives us an equation for the radius. Dividing column 1 of the determinant by $\sin k_1 a$, column 2 by $\sinh k_2 a$, column 3 by $e^{-v_1 a}$, column 4 by $e^{-v_2 a}$, multiplying row 1 by a, and row 3 by 2 gives the following equation for a.

[redacted]

[redacted]

$$
\begin{vmatrix}
1 & 1 & 1 & 1 \\
\alpha_o\left[\dfrac{\cot k_1a}{k_1a} - \dfrac{1}{k_1^2a^2}\right] & -\alpha_o\left[\dfrac{\coth k_2a}{k_2a} - \dfrac{1}{k_2^2a^2}\right] & \alpha_o'\left(\dfrac{1}{v_1a} + \dfrac{1}{v_1^2a^2}\right) & \alpha_o'\left(\dfrac{1}{v_2a} + \dfrac{1}{v_2^2a^2}\right) \\
c_1\left[\left(1 - \dfrac{3}{k_1^2a^2}\right) + \dfrac{3\cot k_1a}{k_1a}\right] & c_3\left[\left(1 + \dfrac{3}{k_2^2a^2}\right) - \dfrac{3\coth k_2a}{k_2a}\right] & c_5\left(1 + \dfrac{3}{v_1a} + \dfrac{3}{v_1^2a^2}\right) & c_7\left(1 + \dfrac{3}{v_2a} + \dfrac{3}{v_2^2a^2}\right) \\
\begin{matrix} c_2\left[\left(\dfrac{2}{k_1^2a^2} - \dfrac{5}{k_1^4a^4}\right)\right. \\ \left. - \left(\dfrac{1}{3k_1a} - \dfrac{5}{k_1^3a^3}\right)\cot k_1a\right] \end{matrix} & \begin{matrix} c_4\left[\left(\dfrac{1}{3k_2a} + \dfrac{5}{k_2^3a^3}\right)\coth k_2a\right. \\ \left. - \left(\dfrac{2}{k_2^2a^2} + \dfrac{5}{k_2^4a^4}\right)\right] \end{matrix} & \begin{matrix} c_6\left(\dfrac{1}{3v_1a} + \dfrac{2}{v_1^2a^2} + \dfrac{5}{v_1^3a^3}\right. \\ \left. + \dfrac{5}{v_1^4a^4}\right) \end{matrix} & \begin{matrix} c_8\left(\dfrac{1}{3v_2a} + \dfrac{2}{v_2^2a^2} + \dfrac{5}{v_2^3a^3}\right. \\ \left. + \dfrac{5}{v_2^4a^4}\right) \end{matrix}
\end{vmatrix} = 0 \qquad (10)
$$

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Setting γ equal to zero (critical) and using the cross sections enumerated above the exact anisotropic solution yields: $a = 1.427 \pm 0.005$ in units of the transport mean free path of the core. Using the transport recipe, 1.430 ± 0.005 is obtained. That is, the two results are indistinguishable.

This extremely close agreement is not surprising when the constants entering into the calculation are examined. Putting the differential equations for the n_ℓ's of the recipe method and of the exact solution in the form (8), we can, by comparing the various α's see by about how much the solutions would be expected to differ (the α's are the only quantities in the two sets of equations which are not identical).

α	Exact Anisotropic Equations	Recipe Equations
α_0	$\gamma - 0.3900$	$\gamma - 0.3900$
α_1	$\gamma + 1.000$	$\gamma + 1$
α_2	$\gamma + 1.1258$	$\gamma + 1$
α_3	$\gamma + 1.1873$	$\gamma + 1$
α_0'	$\gamma + 0.0414$	$\gamma + 0.0414$
α_1'	$\gamma + 1.3515$	$\gamma + 1.3515$
α_2'	$\gamma + 1.411$	$\gamma + 1.3515$
α_3'	$\gamma + 1.4711$	$\gamma + 1.3515$

We note that the quantities to which the calculations are most sensitive ($\alpha_0, \alpha_1, \alpha_0', \alpha_1'$) are exactly right, while even the higher α's (which are in the nature of corrections themselves) are never very far off. In fact it is easily shown that the equality found must be true in general. Thus for the exact solution: $\alpha_0 = \gamma + \sigma_t - \sigma_0 - \nu\sigma_f$. But

$$\gamma_d = \int_{-1}^{1} \sigma_s(\theta)\, d\mu$$

This yields: $\sigma_t = \sigma_o + \sigma_r + \sigma_f$ and

$$\alpha_o = \gamma + \sigma_o + \sigma_r + \sigma_f - \sigma_o - \nu\sigma_f = \gamma + \sigma_r + (1-\nu)\sigma_f$$

The recipe solution gives: $\alpha_o = \gamma - f$, but in our units $f = (\nu-1)\sigma_f - \sigma_r$

and so: $\alpha_o = \gamma + \sigma_r + (1-\nu)\sigma_f$ -- exactly the same as above.

For α_1 the correct solution gives:

$$\alpha_1 = \sigma_t - \sigma_1 + \gamma. \qquad \sigma_1 = \int_{-1}^{1} \mu\, \sigma_s(\theta)\, d\mu \quad \text{and}$$

$$\sigma_t = \int_{-1}^{1} \sigma_s(\theta)\, d\mu + \sigma_f + \sigma_r. \quad \text{This leads to}$$

$$\alpha_1 = \gamma + \sigma_f + \sigma_r + \int_{-1}^{1} (1 - \cos\theta)\, \sigma_s(\theta)\, d(\cos\theta)$$

or

$$\alpha_1 = \gamma + \sigma_{tr} = \gamma + 1 \qquad \text{(in our units).}$$

This last is just the α_1 given by the recipe. Exactly similar considerations prove that α_o' and α_1' are given correctly by the recipe. (This is, of course, the well-known result of differential diffusion theory.)

From the table useful information as to the results that would be obtained with γ's greater than zero (i.e., multiplying media) can be estimated. It can be seen that with increasing γ the percentage difference between the two sets of constants decreases. This would indicate that for $\gamma > 0$ it could be expected that the results obtained by the two methods would be even closer than those found for $\gamma = 0$.

In concluding, the following remarks can be made. It is but slightly more trouble to include angular dependence of the scattering cross section than to leave it out. On the other hand, the simple recipe of substituting the transport cross section whenever the total cross section appears in the equations gives

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results that are identical with the correct method for all practical purposes. Certainly considering the accuracy with which other quantities involved in critical-mass calculations, such as cross sections, are known any error introduced by using the simple recipe is completely negligible.

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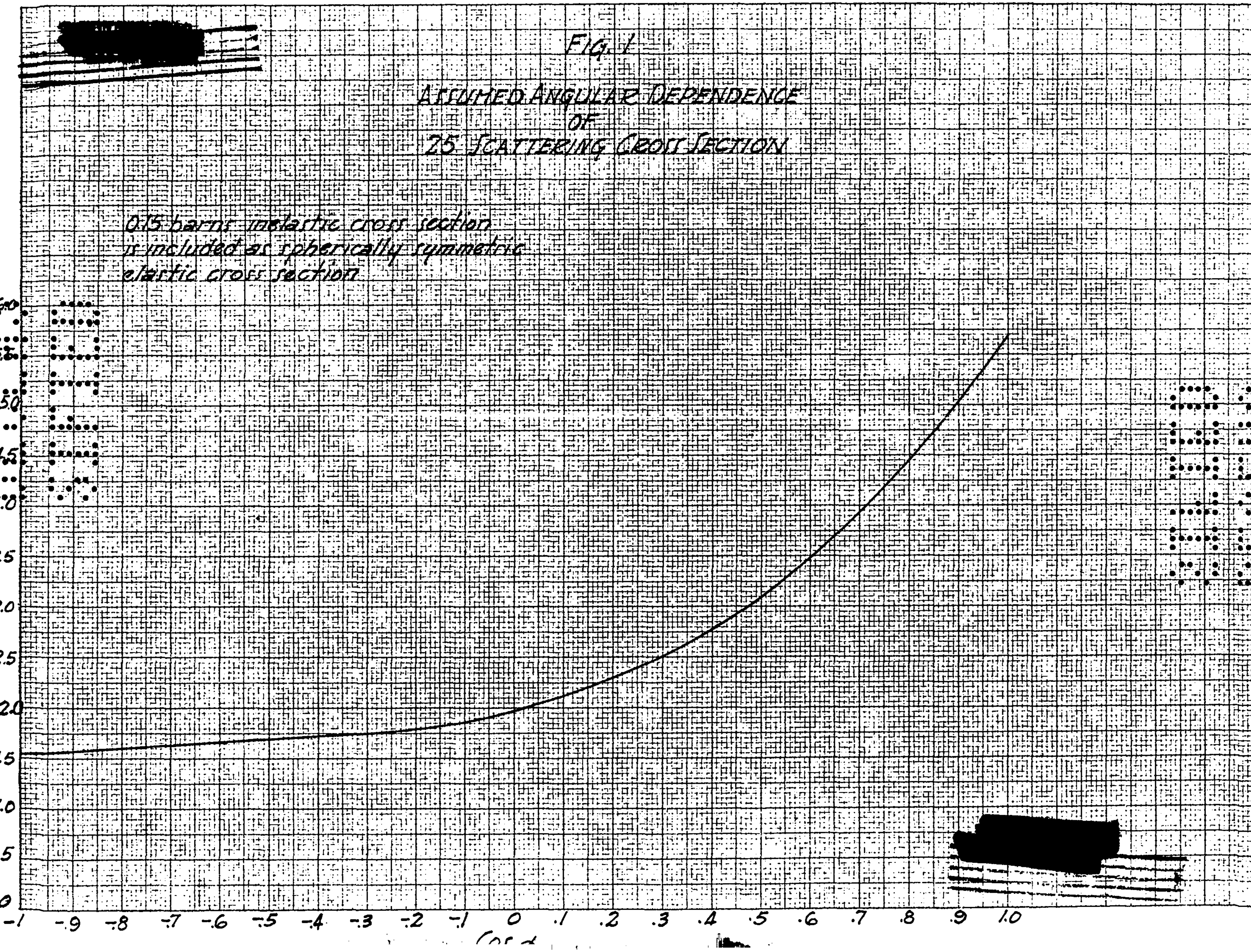

FIG. 1

ASSUMED ANGULAR DEPENDENCE OF 25 SCATTERING CROSS SECTION

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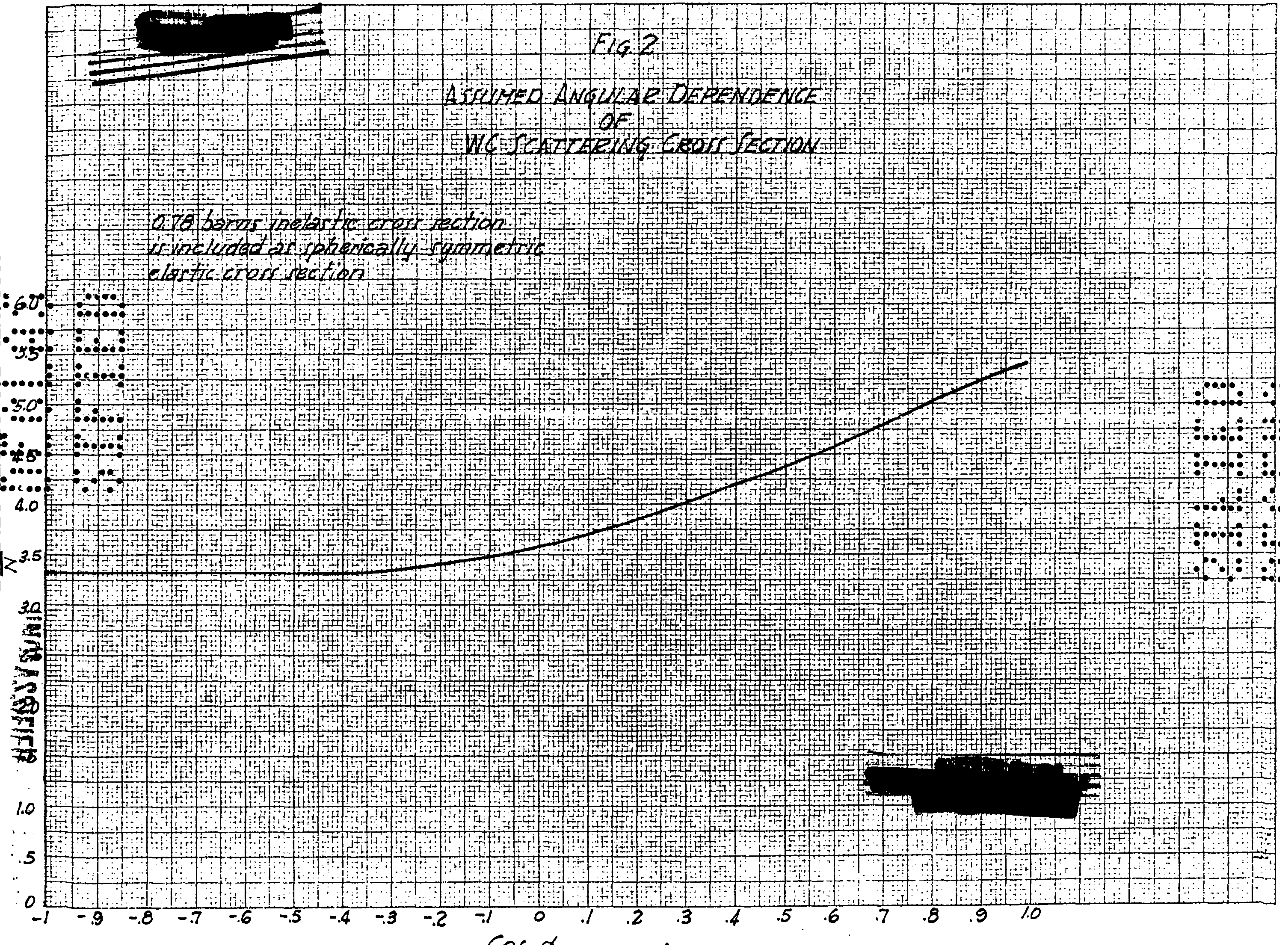

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